



UCMR 3 Chemical Contaminants – Information Compendium

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Contents

Introduction.....	1
17- β -Estradiol.....	5
17- α -Ethinylestradiol	9
Estriol	13
Equilin	15
Estrone	17
Testosterone	21
4-Androstene-3,17-dione.....	23
1,2,3-Trichloropropane	25
1,3-Butadiene.....	29
Chloromethane (Methyl chloride)	31
1,1-Dichloroethane.....	35
Bromomethane (Methyl bromide).....	39
Chlorodifluoromethane (HCFC-22)	45
Bromochloromethane (Halon 1011).....	47
1,4-Dioxane.....	51
Vanadium	53
Molybdenum.....	55
Cobalt.....	57
Strontium	61
Chlorate	65
Perfluorooctanesulfonic Acid (PFOS).....	67
Perfluorooctanoic Acid (PFOA)	71
Perfluorononanoic Acid (PFNA).....	75
Perfluorohexanesulfonic Acid (PFHxS).....	79
Perfluoroheptanoic Acid (PFHpA)	83
Perfluorobutanesulfonic Acid (PFBS)	85
Chromium (total) (regulated)	87
Chromium-6 (Hexavalent Chromium)	87
Appendix A – Persistence and Mobility.....	91
Appendix B – List of Chemical Contaminants Considered for Inclusion on UCMR 3	93
Appendix C – Proposed Contaminants Removed for the Final UCMR 3	99
<i>sec</i> -Butylbenzene.....	101
<i>n</i> -Propylbenzene.....	105

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Introduction

The 1996 amendments to the Safe Drinking Water Act (SDWA) (section 1445) require the United States Environmental Protection Agency (EPA) to promulgate regulations for the monitoring of unregulated contaminants. The 1996 SDWA amendments specify that EPA develop a new list of not more than 30 contaminants every 5 years for public water system (PWS) monitoring. The general structure of the Unregulated Contaminant Monitoring Regulation (UCMR) program was established during the first UCMR (UCMR 1: 2001 – 2005), and divided the contaminants among three separate monitoring program components, related in part to the availability, cost, and efficacy of analytical methods. The second UCMR (UCMR 2: 2007 – 2011) has just been completed. EPA published “Revisions to the Unregulated Contaminant Monitoring Regulation for Public Water Systems; Proposed Rule,” on March 3, 2011.

In establishing its proposed list of contaminants for the third UCMR (UCMR 3), EPA used a stepwise prioritization process similar to the process used for UCMR 1 and 2. As a first step, the agency reviewed the recently promulgated CCL 3 and the “pre-CCL” contaminants considered in the development of CCL 3. Under the CCL 3 process, the agency considered the best available data and information on health effects and occurrence to evaluate 7,500 unregulated contaminants. The final CCL 3 is comprised of 104 chemicals or chemical groups and 12 microbiological contaminants that were selected through a data-driven process that considered adverse health effects (potency and severity) and occurrence (prevalence and magnitude). The list includes pesticides, biological toxins, disinfection byproducts, chemicals used in commerce, and waterborne pathogens (74 FR 51850, October 8, 2009 [USEPA, 2009]). EPA used CCL 3, along with additional sources of information about other emerging contaminants of concern, to establish an initial list of almost 150 potential UCMR 3 contaminants.

Appendix B, “List of Chemical Contaminants Considered for Inclusion on UCMR 3”, presents the initial list of contaminants that EPA considered and identifies which contaminants were listed as part of CCL 3 or other CCL/UCMR lists. The last column of the Appendix B table indicates the reason each contaminant was eliminated from UCMR3 consideration, if applicable. The proposed contaminant list for UCMR 3 was pared down as follows: (1) contaminants with no currently available methods, or methods that would not be ready in time for UCMR 3 monitoring, were eliminated and (2) those contaminants included in UCMR 1 or UCMR 2 monitoring were eliminated from inclusion. This narrowed list of fewer than 35 analytes was further considered by an EPA and state working group, and prioritized using health effects data and other critical endpoints, to arrive at a proposed list of 28 chemical analytes. In addition, 2 microbial analytes (enterovirus and norovirus) were proposed for inclusion in UCMR 3. The viruses are addressed in more detail in the proposed and final rule preambles.

Following publication of the March 2011 proposed rule, EPA received input from 53 public commenters. While EPA did not include chromium-6 in the proposed list of chemicals for UCMR 3 monitoring, EPA did specifically request comment on whether it should be included in the final rule due to concerns about its potential occurrence in public water supplies. EPA also requested comments on whether total chromium should be measured concurrent with chromium-6. Commenters strongly supported requiring monitoring for both chromium-6 and total chromium. After considering the comments, EPA added chromium-6 to UCMR 3, List 1. EPA is using the authority provided in SDWA Section 1445(a)(1)(A) to require monitoring for total chromium in

conjunction with the UCMR 3 monitoring of chromium-6. In addition, EPA removed *sec*-butylbenzene and *n*-propylbenzene. The 28 UCMR 3 chemical contaminants are listed in Exhibit 1a and 1b, below.

This document contains information sheets for the UCMR 3 chemical contaminants. Information sheets for *sec*-butylbenzene and *n*-propylbenzene can be found in “Appendix C – Proposed Contaminants Removed for the Final UCMR 3”. This information was compiled by EPA for consideration and comparison of critical endpoints, as well as to provide information to interested stakeholders. The primary source of this information is CCL 3. In addition, preliminary occurrence data that were collected as part of EPA’s second Six-Year Review of National Primary Drinking Water Regulations (75 FR 15500, March 29, 2010 [USEPA, 2010]) are included. Where newer or additional information was available, and for those contaminants that were not part of CCL 3, references are provided separately. Information for each of the chemicals generally includes five sections:

- **Background & Use** – includes, where available: analyte use, chemical class, and synonym information.
- **Health Effects** – includes, where available: Reference Dose (RfD), Minimal Risk Level (*Minimal Risk Level (MRL)*), No Observed Adverse Effect Level (NOAEL), Lowest Observed Adverse Effect Level (LOAEL), slope factor, Acceptable Daily Intake (ADI), and cancer class data. Non-cancer data are generally presented and grouped first in this section; cancer data second. Also presented are non-cancer and cancer Health Reference Levels (HRLs), which are derived based on key health endpoints.
- **Production & Release** – includes, where available: National Center for Food and Agricultural Policy (NCFAP) Pesticide Use Database, United States Geological Survey (USGS) Pesticide Use Maps, Chemical Update System/Inventory Update Rule (CUS/IUR), Toxics Release Inventory (TRI), estimated usage published in the Office of Pesticide Programs Reregistration Eligibility Decision (OPP RED), and High Production Volume (HPV) data.
- **Occurrence in Water** – includes, where available: raw and finished drinking water and ambient water data.
- **Persistence & Mobility** – includes, where available: water solubility, organic carbon partitioning coefficient (K_{oc}), octanol-water partitioning coefficient ($\log K_{ow}$), Henry’s law constant (K_H), Percent in Water in a Water/Air/Soil/Sediment System (W%) (PBT Profiler), and estimated biodegradation half-life data (see Appendix A for further explanation of the mobility scales developed and used by the CCL 3 workgroup).

Exhibit 1a: UCMR 3 Final Chemical Contaminant Lists	
List 1, Assessment Monitoring¹	
1,4-dioxane	vanadium
molybdenum	strontium
cobalt	chromium-6 (hexavalent chromium) ²
1,2,3-trichloropropane	chlorate
1,3-butadiene	perfluorooctanesulfonic acid (PFOS)
chloromethane (methyl chloride)	perfluorooctanoic acid (PFOA)
1,1-dichloroethane	perfluorononanoic acid (PFNA)
bromochloromethane (Halon 1011)	perfluorohexanesulfonic acid (PFHxS)
bromomethane (methyl bromide)	perfluoroheptanoic acid (PFHpA)
chlorodifluoromethane (HCFC-22)	perfluorobutanesulfonic acid (PFBS)
List 2, Screening Survey³	
17- β -estradiol	estriol
17- α -ethynylestradiol (ethinyl estradiol)	equilin
estrone	testosterone
4-androstene-3,17-dione	
Exhibit 1b: Total Chromium Monitoring⁴	
total chromium	

1. Assessment Monitoring (List 1); includes contaminants measured with common analytical method technologies used by drinking water laboratories.

2. Chromium-6 will be measured as soluble chromate (ion).

3. Screening Survey (List 2); includes contaminants measured using specialized analytical method technologies not as commonly used by drinking water laboratories.

4. Monitoring for total chromium – in conjunction with UCMR 3 Assessment Monitoring – is required under the authority provided in Section 1445(a)(1)(A) of SDWA.

References

USEPA. 2009. Drinking Water Contaminant Candidate List 3–Final. *Federal Register*. Vol. 74, No. 194, p. 51850, October 8, 2009.

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UCMR 3 Analyte Information Sheet

17- β -Estradiol

CASRN: 50-28-2

Background & Use

- 17- β -Estradiol is an estrogenic hormone naturally produced within the human body, and used in pharmaceuticals products.
- Names & Synonyms: 17- β -Estradiol; estradiol; oestradiol; E2.
- 17- β -Estradiol is one of 104 currently unregulated chemicals on CCL 3.
- Research has indicated that oxidative treatment of aqueous solutions of 17- β -estradiol with sodium hypochlorite results in a reduction in the estrogenic activity of the solution after two to three hours (Hu et al., 2003).

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (Minimal Risk Level (MRL))*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: 39 (mg/kg/day)⁻¹ (*California Office of Environmental Health and Hazard Assessment [OEHHA] Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: 0.00005 mg/kg/day, associated with estrogenic hormonal response in post-menopausal women (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] ADI*).
- *Cancer and/or Teratogen Class*:
 - 1 – the agent is carcinogenic to humans (*International Agency for Research on Cancer (IARC) Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*:
 - 0.35 μ g/L for non-cancer effects in drinking water based on the JECFA ADI of 0.00005 mg/kg/day.
 - 0.009 μ g/L for cancer effects in drinking water based on the OEHHA oral slope factor of 39 (mg/kg/day)⁻¹ (*set at 10⁻⁵ risk level*).

Production & Release

- No data for production and release.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: no ground water data were reported.
 - Surface Water: detects in 14 (7.45%) of 188 samples; detects were from 14 (10.77%) of the 130 sites; detects were from 2 states; detects ranged from 0 – 2,210 µg/L.
- *Colorado Surface Water (2000)*: not detected in 8 samples; wastewater effluent samples were excluded (Barber et al., 2003).
- *Louisiana Raw and Finished Waters (2001)*: not detected in 4 samples (Boyd et al., 2003).
- *Chesapeake Bay Tributaries (2004)*: detects in 6 (100%) of 6 Chesapeake Bay water samples at concentrations ranging from 0.0023 – 0.0032 µg/L; detects in 3 (100%) of 3 pond samples at concentrations ranging from 0.0017 – 0.0076 µg/L; detects in 6 (100%) of 6 river samples at concentrations ranging from 0.0019 – 0.006 µg/L (Dorabawila and Gupta, 2005).
- *Missouri Surface Water (2004 – 2005)*: reported detections ranged from 0.0016 – 0.0198 µg/L with a median concentration of 0.00576 µg/L; note that the number of detects in 25 samples was not reported (Filali-Meknassi et al., 2007).
- *California Surface Water (1999)*: detected at 3 (100%) of the 3 sites at concentrations ranging from 0.00005 – 0.0008 µg/L and a median concentration of 0.00008 µg/L (Huang and Sedlak, 2001).
- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 7 (10%) of 70 samples using one method at a median concentration of 0.009 µg/L and a maximum concentration of 0.093 µg/L; detects in 9 (10.6%) of 85 samples using another method at a median concentration of 0.16 µg/L and a maximum concentration of 0.2 µg/L (Kolpin et al., 2002).
- *California, Rivers, Irrigation Canals, and Tile Drains (2003 – 2005)*: detects in 1 (9%) of 11 river samples at a concentration of 0.0006 µg/L; detects in 1 (7%) of 15 irrigation canal samples at a concentration of 0.0007 µg/L; not detected in 6 tile drain samples (Kolodziej et al., 2004).
- *New York City Surface Water (2003 – 2004)*: not detected in 368 samples (Palmer et al., 2008).
- *California, Runoff from Agricultural Fields Irrigated with Treated Wastewater (1999 – 2000)*: number of detects not reported; concentration of detects in runoff samples 0.003 µg/L; concentration of detects in stream samples < 0.47 µg/L (Pedersen et al., 2005).
- *Michigan and Nevada Surface Water (1997)*: detected at 4 (60%) of the 6 Lake Mead sites at concentrations ranging from 0.188 – 2.67 µg/L; detected at 4 (80%) of the 5 Trenton Channel sites (point source locations excluded) at concentrations ranging from 0.435 – 1.29 µg/L; detected at 1 (33%) of the 3 Michigan surface water sites (effluent locations excluded) at a concentration of 0.711 µg/L (Snyder et al., 1999).
- *American Water Works Association National Study*: not detected in either finished drinking water or raw drinking water from 20 drinking water utilities (Snyder et al., 2007).
- *U.S. Raw and Finished Water*: not detected in either finished drinking water or raw drinking water samples from 20 drinking water utilities (Snyder, 2008).
- *National Occurrence of EDCs in Water*: detects in 1 (5%) raw water sample taken from 19 sites at a concentration of 0.017 µg/L; detects in 2 (11%) source water samples taken from 18 sites at a

maximum concentration of 0.002 µg/L and a median concentration of 0.0014 µg/L; not detected in 18 finished water or 15 distribution water sites (Snyder et al., 2008).

- *Nebraska, Water Bodies Receiving Cattle Feedlot Effluent (2000)*: detected at 1 (100%) of 1 sites at 0.000084 µg/L using immunometric method (EIA); the retention pond (site 1) data was excluded (Soto et al., 2004).
- *Massachusetts, Groundwater Affected by Residential Septic System on Cape Cod (2003 – 2004)*: at 9 down gradient locations detects in 10 (71%) of 14 samples at concentrations ranging from 0.0002 – 0.045 µg/L (Swartz et al., 2006).
- *Nevada Surface Water*: not detected in 9 Las Vegas Wash or Lake Mead samples (Vanderford et al., 2003).

Persistence & Mobility

- *Water Solubility*: 3.6 mg/L, indicates 17-β-estradiol is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 4.01, indicates 17-β-estradiol is not very mobile in water.
- *Henry's Law Constant (K_H)*: 3.64E-11 atm·m³/mol, indicates 17-β-estradiol is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 11% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates 17-β-estradiol is moderately persistent in the environment.

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UCMR 3 Analyte Information Sheet

17- α -Ethinylestradiol

CASRN: 57-63-6

Background & Use

- 17- α -Ethinylestradiol is a synthetic estrogenic hormone and is used in veterinary and human pharmaceuticals.
- Names & Synonyms: 17- α -Ethinylestradiol; ethinyl estradiol; EE2; ethinyl E2; estra-1,3,5(10)-triene-3,17 β -diol, 17 α -ethinyl-.
- 17- α -Ethinylestradiol is one of 104 chemicals on CCL 3.
- Research has indicated that oxidative treatment of aqueous solutions of 17- α -ethinylestradiol with chlorine, bromine, ozone, hydroxyl radical, chlorine dioxide, or ferrate ion results in a rapid reduction in the estrogenic activity of the solution (Lee et al., 2008).

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: 0.04 mg/kg/day, associated with hematological effects (*Supplemental NOAEL*).
- *Lowest Observed Adverse Effect Level (LOAEL)*: 0.015 mg/kg/day, associated with increased serum levels of alanine aminotransferase (ALT), aspartate aminotransferase (AST), and γ -glutamyltransferase (GGT) (*Supplemental LOAEL*).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 0.035 μ g/L for non-cancer effects in drinking water based on the Supplemental LOAEL of 0.015 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.

- Ground Water: no ground water data were reported.
- Surface Water: detects in 3 (100.00%) of 3 samples; detects were from all 3 (100.00%) of the sites that reported data; detects were from 1 state; detects were all equal to 0.01 µg/L.
- *Colorado Surface Water (2000)*: not detected in 8 samples; wastewater effluent samples were excluded (Barber et al., 2003).
- *Missouri Surface Water (2004 – 2005)*: reported detections ranged from 0.0013 – 0.0116 µg/L with a median concentration of 0.00265 µg/L; note that the number of detects in 25 samples was not reported (Filali-Meknassi et al., 2007).
- *California Surface Water (1999)*: detected at 1 (33%) of the 3 sites at a concentration of 0.07 µg/L (Huang and Sedlak, 2001).
- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 4 (5.7%) of 70 samples at a median concentration of 0.094 µg/L and a maximum concentration of 0.273 µg/L (Kolpin et al., 2002).
- *New York City Surface Water (2003 – 2004)*: not detected in 240 samples (Palmer et al., 2008).
- *Michigan and Nevada Surface Water (1997)*: detected at 3 (50%) of the 6 Lake Mead sites at concentrations ranging from 0.253 – 0.52 ± 0.117 µg/L; detected at 1 (20%) of the 5 Trenton Channel sites (point source locations excluded) at a concentration of 0.359 µg/L; detected at 0 (0%) of the 3 Michigan surface water sites (effluent locations excluded) (Snyder et al., 1999).
- *American Water Works Association National Study*: not detected in either finished drinking water or raw drinking water from 20 drinking water utilities (Snyder et al., 2007).
- *U.S. Raw and Finished Water*: not detected in either finished drinking water or raw drinking water samples from 20 drinking water utilities (Snyder, 2008).
- *National Occurrence of EDCs in Water*: detects in 1 (5%) raw water sample taken from 19 sites at a concentration of 0.0014 µg/L; not detected at 18 source water, 18 finished water, or 15 distribution water sites (Snyder et al., 2008).
- *Nebraska, Water Bodies Receiving Cattle Feedlot Effluent (2000)*: detected at 1 (100%) of 1 sites at a concentration of 0.000026 µg/L using GC/MS and 0.000035 µg/L using immunometric method (EIA); the retention pond data were excluded (Soto et al., 2004).
- *Nevada Surface Water*: not detected in 9 Las Vegas Wash or Lake Mead samples (Vanderford et al., 2003).

Persistence & Mobility

- *Water Solubility*: 11.3 mg/L, indicates 17- α -ethynylestradiol is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 3.67, indicates 17- α -ethynylestradiol is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 7.94E-12 atm-m³/mol, indicates 17- α -ethynylestradiol is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 9% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 60 days, indicates 17- α -ethynylestradiol is persistent in the environment.

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UCMR 3 Analyte Information Sheet

Estriol

CASRN: 50-27-1

Background & Use

- Estriol is an estrogenic hormone naturally produced within the human body, and is used in pharmaceuticals products
- Names & Synonyms: 16- α -Hydroxyestradiol; E3; estratriol; oestriol; 16- α -hydroxy-17- β -estradiol.
- Estriol is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 0.00005 mg/kg/day, associated with estrogenic hormonal response in post-menopausal women. ADI for 17- β -estradiol (E2); E2 has structural similarities to estriol, so used as a toxicological surrogate (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] Acceptable Daily Intake [ADI]*).
- *Cancer and/or Teratogen Class*: Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 0.35 μ g/L for non-cancer effects in drinking water based on the JECFA ADI of 0.00005 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *Colorado Surface Water (2000)*: detects in 1 (12.5%) of 8 samples at a maximum concentration of 0.0031 μ g/L; wastewater effluent samples were excluded (Barber et al., 2003).
- *Missouri Surface Water (2004 – 2005)*: reported detections ranged from 0.0007 – 0.0048 μ g/L with a median concentration of 0.00124 μ g/L; note that the number of detects in 25 samples was not reported (Filali-Meknassi et al., 2007).
- *California Ground and Surface Waters (2003 – 2004)*: not detected in surface or ground water samples (Kolodziej et al., 2004).

- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 15 (21.4%) of 70 samples at a median concentration of 0.019 µg/L and a maximum concentration of 0.051 µg/L (Kolpin et al., 2002).
- *American Water Works Association National Study*: not detected in either finished drinking water or raw drinking water from 20 drinking water utilities (Snyder et al., 2007).

Persistence & Mobility

- *Water Solubility*: 441 mg/L, indicates estriol is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 2.45, indicates estriol is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 1.33E-12 atm-m³/mol, indicates estriol is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 17% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates estriol is moderately persistent in the environment.

References

Barber, L.B., E.T. Furlong, S.H. Keefe, G.K. Brown, and J.D. Cahill. 2003. *Chapter 5 – Natural and Contaminant Organic Compounds in the Boulder Creek Watershed, Colorado During High-Flow and Low-Flow Conditions, 2000*.

Filali-Meknassi, Y., M. Auriol, C.D. Adams, and R.Y. Surampalli. 2007. Quantification of steroid sex hormones using solid-phase extraction followed by liquid chromatography-mass spectrometry. *Water Environment Research*. 79(6): 687-695.

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Snyder, A.S., E.C. Wert, H. Lei, P. Westerhoff, and Y. Yoon. 2007. *Removal of EDCs and Pharmaceuticals in Drinking and Reuse Treatment Processes*. American Water Works Association.

UCMR 3 Analyte Information Sheet

Equilin

CASRN: 474-86-2

Background & Use

- Equilin is an estrogenic hormone derived from horses, and is used in pharmaceuticals products
- Names & Synonyms: Equilin; 7-dehydroestrone; dihydroequilenin; 3-hydroxyestra-1,3,5,7-tetraen-17-one.
- Equilin is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 0.00005 mg/kg/day, associated with estrogenic hormonal response in post-menopausal women. ADI for 17- β -estradiol (E2); E2 has structural similarities to equilin, so used as a toxicological surrogate. (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] Acceptable Daily Intake [ADI]*).
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 0.35 μ g/L for non-cancer effects in drinking water based on the JECFA ADI of 0.00005 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: no ground water data were reported.
 - Surface Water: detects in 3 (7.32%) of 41 samples; detects were from 3 (13.04%) of the 23 sites; detects were from 1 state; detects were all equal to 0.01 μ g/L.
- *Colorado Surface Water (2000)*: not detected in 8 samples; wastewater effluent samples excluded (Barber et al., 2003).

- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 1 (1.4%) of 70 samples at a concentration of 0.147 µg/L (Kolpin et al., 2002).

Persistence & Mobility

- *Water Solubility*: 1.41 mg/L, indicates equilin is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 3.35, indicates equilin is moderately mobile in water.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 13% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates equilin is moderately persistent in the environment.

References

Barber, L.B., E.T. Furlong, S.H. Keefe, G.K. Brown, and J.D. Cahill. 2003. *Chapter 5 – Natural and Contaminant Organic Compounds in the Boulder Creek Watershed, Colorado During High-Flow and Low-Flow Conditions, 2000*.

Kolpin, D.W., E.T. Furlong, M.T. Meyer, E.M. Thurman, S.D. Zaugg, L.B. Barber, and H.T. Buxton. 2002. Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999-2001: A national reconnaissance. *Environmental Science and Technology*. 36: 1202-1211.

UCMR 3 Analyte Information Sheet

Estrone

CASRN: 53-16-7

Background & Use

- Estrone is an estrogenic hormone naturally produced within the human body, and is used in pharmaceuticals products.
- Names & Synonyms: Estrone; estrol; esterone; E1.
- Estrone is one of 104 chemicals on the CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 0.00005 mg/kg/day, associated with estrogenic hormonal response in post-menopausal women. ADI for 17- β -estradiol (E2); E2 has structural similarities to estrone, so used as a toxicological surrogate (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] Acceptable Daily Intake [ADI]*).
- *Cancer and/or Teratogen Class*:
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 0.35 μ g/L for non-cancer effects in drinking water based on the JECFA ADI of 0.00005 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: no ground water data were reported.
 - Surface Water: detects in 3 (7.32%) of 41 samples; detects were from 3 (13.04%) of the 23 sites; detects were from 1 state; detects were all equal to 0.01 μ g/L.

- *Colorado Surface Water (2000)*: not detected in 8 samples; wastewater effluent samples were excluded (Barber et al., 2003).
- *Southeastern Louisiana, Mississippi River and Lake Pontchartrain Surface Water (2000)*: detected at 7 (100%) of the 7 sites (4 samples were collected at each site) at a median concentration range of < 0.01 – 0.02 µg/L (Boyd and Grimm, 2001).
- *Louisiana Raw and Finished Waters (2001)*: not detected in 4 samples (Boyd et al., 2003).
- *Missouri Surface Water (2004 – 2005)*: reported detections ranged from 0.0006 – 0.0155 µg/L with a median concentration of 0.00127 µg/L; note that the number of detects in 25 samples was not reported (Filali-Meknassi et al., 2007).
- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 5 (7.1%) of 70 samples at a median concentration of 0.027 µg/L and a maximum concentration of 0.112 µg/L (Kolpin et al., 2002).
- *California, Rivers, Irrigation Canals, and Tile Drains (2003 – 2005)*: detects in 5 (45%) of 11 river samples at a maximum concentration of 0.0009 µg/L; detects in 7 (47%) of 15 irrigation canal samples at a maximum concentration of 0.017 µg/L; not detected in 6 tile drain samples (Kolodziej et al., 2004).
- *New York City Surface Water (2003 – 2004)*: detects in 1 (0.3%) of 368 samples at a concentration of 0.056 µg/L (Palmer et al., 2008).
- *California, Runoff from Agricultural Fields Irrigated with Treated Wastewater (1999 – 2000)*: number of detects not reported; concentration of detects in runoff samples 0.052 µg/L; concentration of detects in stream samples < 0.2 µg/L (Pedersen et al., 2005).
- *American Water Works Association National Study*: detects in 2 (10%) of 20 drinking water utilities finished and raw drinking waters samples; finished drinking water concentrations ranged from 0.0011 – 0.0023 µg/L with a median concentration of 0.0017 µg/L; raw drinking water concentrations ranged from 0.001 – 0.0014 µg/L with a median concentration of 0.0012 µg/L (Snyder et al., 2007).
- *U.S. Raw and Finished Water*: detects in 74% of raw water samples from 20 drinking water utilities at a maximum concentration of 0.002 µg/L and a median concentration of 0.0004 µg/L; not detected in finished water samples from 20 drinking water utilities (Snyder, 2008).
- *National Occurrence of EDCs in Water*: detects in 15 (79%) raw water samples taken from 19 sites at a maximum concentration of 0.00094 µg/L and a median concentration of 0.00033 µg/L; detects in 11 (61%) source water samples taken from 18 sites at a maximum concentration of 0.0062 µg/L and a median concentration of 0.0012 µg/L; not detected at 18 finished water or 15 distribution water sites (Snyder et al., 2008).
- *Nebraska, Water Bodies Receiving Cattle Feedlot Effluent (1999, 2000)*: detected at 5 (100%) of the 5 sites in 1999 at concentrations ranging from < 0.00021 – 0.0016 µg/L using immunometric method (EIA) and 0.000246 – 0.002164 µg/L using GC/MS; detected at 1 (100%) of 1 sites in 2000 at 0.0009 µg/L using EIA and 0.002434 µg/L using GC/MS; the retention pond (site 1) data were excluded (Soto et al., 2004).
- *Massachusetts, Groundwater Affected by Residential Septic System on Cape Cod (2003 – 2004)*: at 9 down gradient locations detects in 10 (71%) of 14 samples at concentrations ranging from 0.0004 – 0.12 µg/L (Swartz et al., 2006).

Persistence & Mobility

- *Water Solubility*: 30 mg/L, indicates estrone is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 3.13, indicates estrone is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 3.80×10^{-10} atm-m³/mol, indicates estrone is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System (W%)*: 13% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates estrone is moderately persistent in the environment.

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- Barber, L.B., E.T. Furlong, S.H. Keefe, G.K. Brown, and J.D. Cahill. 2003. *Chapter 5 – Natural and Contaminant Organic Compounds in the Boulder Creek Watershed, Colorado During High-Flow and Low-Flow Conditions, 2000*.
- Boyd, G.R. and D.A. Grimm. 2001. Occurrence of pharmaceutical contaminants and screening of treatment alternatives for southeastern Louisiana. *Annals New York Academy of Science*. 80-89.
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- Filali-Meknassi, Y., M. Auriol, C.D. Adams, and R.Y. Surampalli. 2007. Quantification of steroid sex hormones using solid-phase extraction followed by liquid chromatography-mass spectrometry. *Water Environment Research*. 79(6): 687-695.
- Kolpin, D.W., E.T. Furlong, M.T. Meyer, E.M. Thurman, S.D. Zaugg, L.B. Barber, and H.T. Buxton. 2002. Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999 – 2000: A national reconnaissance. *Environmental Science and Technology*. 36(6): 1202-1211.
- Kolodziej, E.P., T. Harter, and D.L. Sedlak. 2004. Dairy wastewater, aquaculture, and spawning fish as sources of steroid hormones in the aquatic environment. *Environmental Science and Technology*. 38: 6377-6384.
- Palmer, P.M., L.R. Wilson, P. O'Keefe, R. Sheridan, T. King, and C-Y. Chen. 2008. Sources of pharmaceutical pollution in the New York City watershed. *Science of the Total Environment*. 394: 90-102.
- Pedersen, J.A., M. Soliman, and I.H. Suffet. 2005. Human pharmaceuticals, hormones, and personal care product ingredients in runoff from agricultural fields irrigated with treated wastewater. *Journal of Agricultural and Food Chemistry*. 53: 1625-1632.
- Snyder, S.A., E.C. Wert, H. Lei, P. Westerhoff, and Y. Yoon. 2007. *Removal of EDCs and Pharmaceuticals in Drinking and Reuse Treatment Processes*. AWWA Research Foundation.
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Soto, A.M., J.M. Calabro, N.V. Precht, A.Y. Yau, E.F. Orlando, A. Daxenberger, A.S. Kolok, L.J. Guillette, B. le Bizec, I.G. Lange, and C. Sonnenschein. 2004. Androgenic and estrogenic activity in water bodies receiving cattle feedlot effluent in eastern Nebraska, USA. *Environmental Health Perspectives*. 112(3): 346-352.

Swartz, C.H., S. Reddy, M.J. Benotti, H. Yin, L.B. Barber, B.J. Brownawell, and R.A. Rudel. 2006. Steroid estrogens, nonylphenol ethoxylate metabolites, and other wastewater contaminants in groundwater affected by a residential septic system on Cape Cod, MA. *Environmental Science and Technology*. 40: 4894-4902.

UCMR 3 Analyte Information Sheet

Testosterone

CASRN: 58-22-0

Background & Use

- Testosterone is an androgenic steroid naturally produced within the human body, and is used in pharmaceuticals products
- Names & Synonyms: Testosterone; teslen; testandron; testobase; testoderm; testosterone; testrone; testryl.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 0.002 mg/kg/day (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] Acceptable Daily Intake [ADI]*).
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 14 µg/L for non-cancer effects in drinking water based on the JECFA ADI of 0.002 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *National Surface Water Reconnaissance (1999 – 2000)*: detects in 2 (2.8%) of 70 samples at a median concentration of 0.116 µg/L and a maximum concentration of 0.214 µg/L (Kolpin et al., 2002).
- *California, Rivers, Irrigation Canals, and Tile Drains (2003 – 2005)*: detects in 2 (18%) of 11 river samples at a maximum concentration of 0.0006 µg/L; detects in 4 (27%) of 15 irrigation canal samples at a maximum concentration of 0.0019 µg/L; detects in 2 (33%) of 6 tile drain samples at a maximum concentration of < 0.0003 µg/L (Kolodziej et al., 2004).
- *City of Ann Arbor Municipal Water Use Cycle (2004)*: not detected in surface/source water, drinking water, wastewater influent, or wastewater effluent samples (Skadsen et al., 2004).
- *American Water Works Association National Study*: not detected in either finished drinking water or raw drinking water from 20 drinking water utilities (Snyder et al., 2007).

Persistence & Mobility

- *Water Solubility*: 23.4 mg/L, indicates testosterone is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 3.32, indicates testosterone is moderately mobile in water.
- *Henry's Law Constant (K_H)*: $3.5\text{E-}09 \text{ atm}\cdot\text{m}^3/\text{mol}$, indicates testosterone is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 14% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates testosterone is moderately persistent in the environment.

References

Kolpin, D.W., E.T. Furlong, M.T. Meyer, E.M. Thurman, S.D. Zaugg, L.B. Barber, and H.T. Buxton. 2002. Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999-2001: A national reconnaissance. *Environmental Science and Technology*. 36: 1202-1211.

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Skadsen, J.M., B.L. Rice, and D.J. Meyering. 2004. *The Occurrence and Fate of Pharmaceuticals, Personal Care Products and Endocrine Disrupting Compounds in a Municipal Water Use Cycle: A Case Study in the City of Ann Arbor*. November 2004.

Snyder, S.A., E.C. Wert, H. Lei, P. Westerhoff, and Y. Yoon. 2007. *Removal of EDCs and Pharmaceuticals in Drinking and Reuse Treatment Processes*. AWWA Research Foundation.

UCMR 3 Analyte Information Sheet

4-Androstene-3,17-dione

CASRN: 63-05-8

Background & Use

- 4-Androstene-3,17-dione is a steroid hormone naturally produced within the human body, and is used as an anabolic steroid and a dietary supplement.
- Names & Synonyms: 4-Androstene-3,17-dione; androstenedione; 3,17-dioxoandrost-4-ene; andro.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 0.002 mg/kg/day. ADI for testosterone; testosterone has structural similarities to 4-androstene-3,17-dione, so used as a toxicological surrogate (*Joint FAO/WHO Expert Committee on Food Additives [JECFA] Acceptable Daily Intake [ADI]*).
- *Cancer and/or Teratogen Class*:
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 14 µg/L for non-cancer effects in drinking water based on the JECFA ADI of 0.002 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *American Water Works Association National Study*: not detected in 20 drinking water utilities finished drinking water; detects in 1 (5%) of 20 drinking water utilities raw drinking water samples at a concentration of 0.0019 µg/L (Snyder et al., 2007).
- *California Surface Waters* (2005 – 2006): detects in 16 (18%) of 89 grazing rangeland surface water samples at a maximum concentration of 0.044 µg/L; not detected in 32 dairy farm surface water samples (Kolodziej and Sedlak, 2007).
- *California, Rivers, Irrigation Canals, and Tile Drains* (2003 – 2005): not detected in 11 river samples, 15 irrigation canal samples, and 6 tile drain samples (Kolodziej et al., 2004).
- *Florida Fenbolloway River* (2001): detected at a concentration of 0.127 µg/L (Debska et al., 2004).

Persistence & Mobility

- *Water Solubility*: 57.2 mg/L, indicates 4-androstene-3,17-dione is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 760 L/kg, indicates 4-androstene-3,17-dione is moderately mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 2.75, indicates 4-androstene-3,17-dione is moderately mobile in water.
- *Henry's Law Constant (K_H)*: $3.70\text{E-}08 \text{ atm-m}^3/\text{mol}$, indicates 4-androstene-3,17-dione is very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 16% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 60 days, indicates 4-androstene-3,17-dione is persistent in the environment.

References

- Debska, J., A. Kot-Wasik, and K. Namiesnik. 2004. Fate and analysis of pharmaceutical residues in the aquatic environment. *Critical Reviews in Analytical Chemistry*. 34: 51-67.
- Kolodziej, E.P. and D.L. Sedlak. 2007. Rangeland grazing as a source of steroid hormones to surface waters. *Environmental Science and Technology*. 41: 3514-3520.
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UCMR 3 Analyte Information Sheet

1,2,3-Trichloropropane

CASRN: 96-18-4

Background & Use

- 1,2,3-Trichloropropane is a halogenated alkane and is used as an ingredient in paint, varnish remover, solvents, and degreasing agents.
- Names & Synonyms: 1,2,3-Trichloropropane; propane, 1,2,3-trichloro-; trichlorohydrin.
- 1,2,3-Trichloropropane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*:
 - 0.006 mg/kg/day, based on a *No Observed Adverse Effect Level (NOAEL)* of 8 mg/kg/day and an Uncertainty Factor (UF) of 1,000, and associated with alterations in clinical chemistry and reduction in Red Blood Cell (RBC) mass in rats (*Integrated Risk Information System [IRIS]*).
 - 0.004 mg/kg/day, based on an adjusted benchmark dose lo ($BMDL_{ADJ}$) of 1.1 mg/kg/day, and associated with increased absolute liver weight in male rats (*IRIS*).
- *Minimal Risk Level (MRL)*: 0.06 mg/kg/day with an Uncertainty Factor (UF) of 100, and associated with hepatic effects (*Agency for Toxic Substances and Disease Registry [ATSDR] Intermediate (MRL)*).
- *NOAEL*: 5.71 mg/kg/day (*Supplemental NOEL*).
- *Lowest Observed Adverse Effect Level (LOAEL)*: 22.9 mg/kg/day, based on a 17-week oral study in rats, and associated with effects on the kidneys, ureters, and bladder, such as changes in bladder weight; effects on the blood, such as changes in serum composition (e.g., TP, bilirubin, cholesterol); biochemical changes, such as enzyme inhibition and induction; and changes in blood or tissue levels (other esterases) (*Registry of Toxic Effects of Chemical Substances [RTECS] Lowest Oral Chronic LOAEL*).
- *Slope Factor*:
 - $7 \text{ (mg/kg/day)}^{-1}$ (*Risk Assessment Information System [RAIS] Oral Slope Factor*).
 - $30 \text{ (mg/kg/day)}^{-1}$ (*IRIS Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: Not Available.
- *Cancer and/or Teratogen Class*: Listed (*State of California List of Chemicals Known to Cause Cancer*).
- *Drinking Water Equivalent Level (DWEL)*: 0.2 mg/L.
- *Health Reference Level (HRL)*:
 - 42 µg/L for non-cancer effects in drinking water based on the IRIS RfD of 0.006 mg/kg/day.
 - 28 µg/L for non-cancer effects in drinking water based on the IRIS RfD of 0.004 mg/kg/day.

- 0.05 µg/L for cancer effects in drinking water based on the RAIS oral slope factor of 7 (mg/kg/day)⁻¹ (*set at the 10⁻⁵ risk level*).
- 0.01 µg/L for cancer effects in drinking water based on the IRIS oral slope factor of 30 (mg/kg/day)⁻¹ (*set at the 10⁻⁵ risk level*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 10 – 50 million pounds in 1998 and > 1 – 10 million pounds in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 4,255 pounds were released into surface water in 1 state, and a total of 98,003 pounds were released into the environment across 2 states.
- *TRI 2004*: facilities reported 282 pounds were released into surface water in 1 state, and a total of 9,053 pounds were released into the environment across 2 states.
- *TRI 2006*: facilities reported 416 pounds were released into surface water in 1 state, and a total of 2,025 pounds were released into the environment across 3 states.
- *High Production Volume (HPV) Challenge Program*: is included in the program which performs baseline testing on chemicals that are made or imported into the U.S. in amounts equal to or greater than one million pounds per year.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 44 (0.25%) of the 17,392 PWSs, at a maximum concentration of 112 µg/L and a median concentration of 0.92 µg/L.
 - Round 2 (1993 – 1997): occurred at 19 (0.08%) of the 24,088 PWSs, at a maximum concentration of 3,000 µg/L and a median concentration of 0.5 µg/L.
- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 38 (2.68%) of 1,420 samples; detects were from 35 (5.25%) of the 667 sites; detects were from 1 state; detects ranged from 0.9 – 10 µg/L.
 - Surface Water: detects in 234 (37.38%) of 626 samples; detects were from 16 (12.31%) of the 130 sites; detects were from 2 states; detects ranged from 0.008 – 0.5 µg/L.
 - Ohio Public Water Supply: not detected in 1,277 drinking water samples from 186 sites that reported data.
- *National Water Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 54 (0.91%) of 5,941 samples and at 43 (1.0%) of the 4,309 sites at a maximum concentration of 2.92 µg/L and a median concentration of 0.4 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)

- Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; detects in 1 (0.1%) of the samples (0.17% of ground water samples and 0% of surface water samples) at a concentration of 0.31 µg/L (Grady, 2003).
- Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 3.8% of the CWSs sampled (3.8% of ground water sites and 3.7% of surface water sites) at concentrations ranging from 0.03 – 0.09 µg/L (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 264 urban wells and 1,729 rural wells; 0.38% detection frequency in urban areas and 0.58% detection frequency in rural areas at concentrations ranging from 0.2 – 1.1 µg/L. In urban wells, the single detection was at a concentration of 0.2 µg/L and in rural wells, the median concentration was 0.5 µg/L (Squillace et al., 1999). (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
- *NAWQA VOCs in Ground Water and Drinking Water Supply Wells (1985 – 2001)*: national assessment comprised of approximately 100 different aquifer studies; roughly 3,500 water samples collected from various types of wells:
 - Aquifers: detects in 17 (0.61%) of 2,765 samples at a median concentration of 0.5 µg/L.
 - Shallow ground water in urban areas: detects in 1 (0.1%) of 847 samples.
 - Shallow ground water in agricultural areas: detects in 7 (1.0%) of 723 samples.
 - Domestic wells: detects in 9 (0.43%) of 2,092 samples at a median concentration of 0.38 µg/L.
 - Public wells: detects in 8 (0.80%) of 997 samples at a median concentration of 0.70 µg/L.
 - Domestic and public wells: detects in 17 (0.6%) of 3,089 samples.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 4,977 (4.40%) of 113,128 drinking water samples; detects were from 157 (3.99%) of the 3,939 PWSs that reported data; detects ranged from 0.001 – 74 µg/L.
 - Illinois: detects in 4 (36.36%) of 11 drinking water samples; detects were from 4 (66.67%) of the 6 CWSs that reported data; detects were all equal to 250 µg/L.
 - North Carolina: detects in 18 (0.09%) of 19,840 drinking water samples; detects were from 5 (0.20%) of the 2,493 PWSs that reported data; detects ranged from 0.57 – 0.8 µg/L.
 - Ohio: detects in 1 (0.01%) of 9,283 drinking water samples at a concentration of 0.5 µg/L; 2,532 PWSs reported data.
 - Region 9 Tribes: detects in 3 (0.27%) of 1,113 drinking water samples; detects were from 2 (0.72%) of the 279 PWSs that reported data; detects ranged from 1.8 – 3.7 µg/L.
 - South Dakota: detects in 1 (0.09%) of 1,110 drinking water samples at a concentration of 0.67 µg/L; 281 PWSs reported data.
 - Texas: detects in 7 (0.02%) of 36,285 drinking water samples; detects were from 5 (0.09%) of the 5,660 PWSs that reported data; detects ranged from 13 – 37 µg/L.
- *Florida Department of Environmental Protection (2004 – 2007)*: detects in 1 (0.06%) of 1,766 drinking water samples at a concentration of 1.9 µg/L; 27 PWSs sampled.

- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 11 (0.08%) of 13,228 drinking water samples; detects were from 11 (0.60%) of the 1,826 PWSs that reported data; detects ranged from 0.1 – 3.21 µg/L.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 1 (0.02%) of 6,462 drinking water samples at a concentration of 3.9 µg/L; 1,123 PWSs reported data.
- *Community Water System Survey (CWSS) (2006)*: 1 system serving > 500,000 people reported monitoring data for 1,2,3-trichloropropane at 400 µg/L.
- *New Jersey Special Study Data (1999 – 2004)*: New Jersey Synthetic Organic Compound (SOC) Waiver Program detected 1,2,3-trichloropropane in excess of health-based drinking water guidance values at 30 (1%) of the 2,640 private wells, and at 11 of the approximately 260 CWSs.

Persistence & Mobility

- *Water Solubility*: 1,750 mg/L, indicates 1,2,3-trichloropropane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 77 – 95 L/kg, indicates 1,2,3-trichloropropane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 2.27, indicates 1,2,3-trichloropropane is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 3.43E-04 atm·m³/mol, indicates 1,2,3-trichloropropane is moderately mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 25% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates 1,2,3-trichloropropane is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

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Squillace, P.J., M.J. Moran, W.W. Lapham, C.V. Price, R.M. Clawges, and J.S. Zogorski. 1999. Volatile Organic Compounds in Untreated Ambient Groundwater of the United States, 1985-1995. *Environmental Science and Technology*. 33(23): 4176-4187.

UCMR 3 Analyte Information Sheet

1,3-Butadiene

CASRN: 106-99-0

Background & Use

- 1,3-Butadiene is an alkene and is used as a chemical in rubber manufacturing and occurs as a gas.
- Names & Synonyms: 1,3-Butadiene; buta-1,3-diene; vinyl ethylene.
- 1,3-Butadiene is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*:
 - $3.4 \text{ (mg/kg/day)}^{-1}$ (*California Office of Environmental Health and Hazard Assessment [OEHHA] Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - B2 – probable human carcinogen (sufficient evidence from animal studies and inadequate/no epidemiologic studies) (*EPA Cancer Class*).
 - 2A – the agent is probably carcinogenic to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: $0.103 \text{ }\mu\text{g/L}$ for cancer effects in drinking water based on the oral slope factor of $3.4 \text{ (mg/kg/day)}^{-1}$ (*set at 10^{-5} risk level*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was > 1 billion pounds in 1998 and in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 2,084 pounds were released into surface water across 8 states, and a total of 1,996,836 pounds were released into the environment across 36 states.
- *TRI 2004*: facilities reported 493 pounds were released into surface water across 8 states, and a total of 2,064,390 pounds were released into the environment across 35 states.

- *TRI 2006*: facilities reported 113 pounds were released into surface water across 7 states, and a total of 2,470,896 pounds were released into the environment across 35 states.

Occurrence in Water

- No data for occurrence in water.

Persistence & Mobility

- *Water Solubility*: 735 mg/L, indicates 1,3-butadiene is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 288 L/kg, indicates 1,3-butadiene is moderately mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 1.99, indicates 1,3-butadiene is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 7.40E-02 atm-m³/mol, indicates 1,3-butadiene is not mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 89% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 7–28 days, indicates 1,3-butadiene is not persistent in the environment.

UCMR 3 Analyte Information Sheet

Chloromethane (Methyl chloride)

CASRN: 74-87-3

Background

- Chloromethane is a halogenated alkane and is used as a foaming agent, in the production of other substances, and is a by-product that can form when chlorine is used to disinfect drinking water.
- Names & Synonyms: Chloromethane; methyl chloride; monochloromethane; methane, chloro-.
- Chloromethane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.004 mg/kg/day, associated with mild neurological effects in humans occupationally exposed to chloromethane (*EPA Health Advisory [HA] RfD*).
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: $0.013 \text{ (mg/kg/day)}^{-1}$ (*Risk Assessment Information System [RAIS] Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
 - 3 – the agent is not classifiable as to its carcinogenicity to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: 0.1 mg/L.
- *Health Reference Level (HRL)*:
 - 28 µg/L for non-cancer effects in drinking water based on the HA RfD of 0.004 mg/kg/day.
 - 26.9 µg/L for cancer effects in drinking water based on the RAIS oral slope factor of $0.013 \text{ (mg/kg/day)}^{-1}$ (*set at the 10^{-5} risk level*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was > 1 billion pounds in 1998 and in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 1,662 pounds were released into surface water across 12 states, and a total of 1,786,609 pounds were released into the environment across 25 states.

- *TRI 2004*: facilities reported 1,539 pounds were released into surface water across 10 states, and a total of 1,761,270 pounds were released into the environment across 26 states.
- *TRI 2006*: facilities reported 10,541 pounds were released into surface water across 8 states, and a total of 1,848,384 pounds were released into the environment across 24 states.
- *High Production Volume (HPV) Challenge Program*: is included in the program which performs baseline testing on chemicals that are made or imported into the U.S. in amounts equal to or greater than one million pounds per year.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 248 (1.22%) of the 20,246 PWSs, at a maximum concentration of 550 µg/L and a median concentration of 1.9 µg/L.
 - Round 2 (1993 – 1997): occurred at 528 (2.25%) of the 23,478 PWSs, at a maximum concentration of 312 µg/L and a median concentration of 1.4 µg/L.
- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 142 (4.00%) of 3,549 samples; detects were from 107 (6.86%) of the 1,560 sites; detects were from 2 states; detects ranged from 0.067 – 10,000 µg/L.
 - Surface Water: detects in 458 (24.12%) of 1,899 samples; detects were from 102 (34.23%) of the 298 sites; detects were from 5 states; detects ranged from 0 – 4.29 µg/L.
 - Ohio Public Water Supply: detects in 4 (0.31%) of 1,276 samples; detects were from 4 (2.15%) of the 186 sites; detects were from 1 (100%) state; detects ranged from 0.6 – 1 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 562 (10.1%) of 5,538 samples and at 356 (8.99%) of the 3,959 sites at a maximum concentration of 21 µg/L and a median concentration of 0.04 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; detects in 3 (0.31%) of the samples (0.52% of ground water samples and 0% of surface water samples) at concentrations ranging from 0.20 – 0.69 µg/L (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 0.7% of the CWSs sampled (1.3% of ground water sites and 0% of surface water sites) at concentrations ranging from 0.11 – 2.63 µg/L. Below the reporting level of 0.2 µg/L, detected at 3.0% of the CWSs sampled (3.8% of ground water sites and 1.8% of surface water sites) (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 189 urban wells and 993 rural wells; 1.06% detection frequency in urban

areas and 0.40% detection frequency in rural areas at concentrations ranging from 0.2 – 21 µg/L. In urban wells, the median concentration was 0.4 µg/L and in rural wells, the median concentration was 0.35 µg/L (Squillace et al., 1999). (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)

- *NAWQA VOCs in Ground Water and Drinking Water Supply Wells (1985 – 2001)*: national assessment comprised of approximately 100 different aquifer studies; roughly 3,500 water samples collected from various types of wells:
 - Aquifers: detects in 34 (1.1%) of 2,988 samples at a median concentration of 0.035 µg/L.
 - Shallow ground water in urban areas: detects in 7 (0.9%) of 804 samples.
 - Shallow ground water in agricultural areas: detects in 1 (0.2%) of 575 samples.
 - Domestic wells: detects in 20 (0.97%) of 2,059 samples at a median concentration of 0.030 µg/L.
 - Public wells: detects in 4 (0.38%) of 1,045 samples at a median concentration of 0.070 µg/L.
 - Domestic and public wells: detects in 24 (0.8%) of 3,104 samples.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 616 (0.55%) of 112,636 drinking water samples; detects were from 142 (3.51%) of the 4,046 PWSs that reported data; detects ranged from 0.25 – 46 µg/L.
 - Illinois: detects in 99 (6.37%) of 1,554 drinking water samples; detects were from 51 (6.90%) of the 739 CWSs that reported data; detects ranged from 0.5 – 25.7 µg/L.
 - North Carolina: detects in 335 (1.69%) of 19,853 drinking water samples; detects were from 222 (8.90%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 24 µg/L.
 - Ohio: detects in 128 (1.38%) of the 9,294 drinking water samples; detects were from 87 (3.43%) of the 2,533 PWSs that reported data; detects ranged from 0.5 – 25 µg/L.
 - Region 9 Tribes: detects in 19 (1.64%) of the 1,160 drinking water samples; detects were from 12 (4.20%) of the 286 PWSs that reported data; detects ranged from 0.6 – 6.1 µg/L.
 - South Dakota: detects in 4 (0.36%) of the 1,110 drinking water samples; detects were from 4 (1.42%) of the 281 PWSs that reported data; detects ranged from 1 – 72 µg/L.
 - Texas: detects in 1,187 (3.26%) of the 36,372 drinking water samples; detects were from 760 (13.43%) of the 5,660 PWSs that reported data; detects ranged from 0.5 – 135 µg/L.
- *Florida Department of Environmental Protection (2004 – 2007)*: detects in 16 (0.90%) of the 1,768 drinking water samples; detects were from 3 (11.54%) of the 26 PWSs that reported data; detects ranged from 0.16 – 72 µg/L.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 330 (2.51%) of the 13,155 drinking water samples; detects were from 226 (12.53%) of the 1,804 PWSs that reported data; detects ranged from 0.07 – 32.6 µg/L.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 119 (1.79%) of the 6,630 drinking water samples; detects were from 78 (6.66%) of the 1,172 PWSs that reported data; detects ranged from 0.11 – 8 µg/L.
- *American Water Works Association Research Foundation (AWWARF)-EPA Study of Disinfection Byproducts (DBPs)*: detects at 1 (8%) of the 12 finished water sites sampled (Krasner et al., 2006).

Persistence & Mobility

- *Water Solubility*: 5,320 mg/L, indicates chloromethane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 14.3 L/kg, indicates chloromethane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 0.91, indicates chloromethane is very mobile in water.
- *Henry's Law Constant (K_H)*: 0.00882 atm-m³/mol, indicates chloromethane is moderately mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 43% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 15 days, indicates chloromethane is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

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UCMR 3 Analyte Information Sheet

1,1-Dichloroethane

CASRN: 75-34-3

Background

- 1,1-Dichloroethane is a halogenated alkane and is used as a solvent.
- Names & Synonyms: 1,1-Dichloroethane; ethane, 1,1-dichloro-; ethylidene chloride.
- 1,1-Dichloroethane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.2 mg/kg/day, based on a No Observed Adverse Effect Level (NOAEL) of 714 mg/kg/day and an Uncertainty Factor (UF) of 3,000, and associated with decreased body weight gain (*Risk Assessment Information System [RAIS]*).
- *Minimal Risk Level (MRL)*: Not available.
- *NOAEL*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: $0.0057 \text{ (mg/kg/day)}^{-1}$ (*California Office of Environmental Health and Hazard Assessment [OEHHA] Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - C – possible human carcinogen (*EPA Cancer Class*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*:
 - 1,400 µg/L for non-cancer effects in drinking water based on the RAIS RfD of 0.2 mg/kg/day.
 - 61.4 µg/L for cancer effects in drinking water based on the oral slope factor of $0.0057 \text{ (mg/kg/day)}^{-1}$ (*set at the 10^{-5} risk level*).
- *CDC's 95th Percentile Concentration*: Less than the detection limit for 1,367 serum samples tested from 2003 – 2004 (Calafat et al., 2007).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 1 – 10 million pounds in 1998 and > 500 thousand – 1 million pounds in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 95 pounds were released into surface water across 3 states, and a total of 103,801 pounds were released into the environment across 3 states.
- *TRI 2004*: facilities reported 63 pounds were released into surface water across 3 states, and a total of 17,368 pounds were released into the environment across 5 states.

- *TRI 2006*: facilities reported 196 pounds were released into surface water across 2 states, and a total of 11,303 pounds were released into the environment across 5 states.
- *High Production Volume (HPV) Challenge Program*: is included in the program which performs baseline testing on chemicals that are made or imported into the U.S. in amounts equal to or greater than one million pounds per year.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 233 (1.14%) of the 20,483 PWSs, at a maximum concentration of 500 µg/L and a median concentration of 1.2 µg/L.
 - Round 2 (1993 – 1997): occurred at 184 (0.74%) of the 24,808 PWSs, at a maximum concentration of 159 µg/L and a median concentration of 1 µg/L.
- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 889 (22.21%) of 4,002 samples; detects were from 263 (15.56%) of the 1,690 sites; detects were from 5 states; detects ranged from 0.1 – 3,600 µg/L.
 - Surface Water: detects in 615 (40.54%) of 1,517 samples; detects were from 86 (26.54%) of the 324 sites; detects were from 4 states; detects ranged from 0 – 1 µg/L.
 - Ohio Public Water Supply: detects in 5 (0.39%) of 1,274 samples; detects were from 3 (1.61%) of the 186 sites; detects were from 1 (100%) state; detects ranged from 0.55 – 2.02 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 221 (3.64%) of 6,072 samples and at 135 (3.10%) of the 4,350 sites at a maximum concentration of 39 µg/L and a median concentration of 0.05 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; detects in 11 (1.2%) of the samples (1.9% of ground water samples and 0% of surface water samples) at concentrations ranging from 0.21 – 10 µg/L (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 5.3% of the CWSs sampled (9.2% of ground water sites and 0% of surface water sites) at concentrations ranging from 0.04 – 3.85 µg/L. Below the reporting level of 0.2 µg/L, detected at 15.9% of the CWSs sampled (26.3% of ground water sites and 1.8% of surface water sites) (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 405 urban wells and 2,539 rural wells; 6.42% detection frequency in urban areas and 0.71% detection frequency in rural areas at concentrations ranging from 0.2 – 39 µg/L. In urban wells, the median concentration was 1.65 µg/L and in rural wells, the median

concentration was 2.3 µg/L (Squillace et al., 1999). (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)

- *NAWQA VOCs in Ground Water and Drinking Water Supply Wells (1985 – 2001)*: national assessment comprised of approximately 100 different aquifer studies; roughly 3,500 water samples collected from various types of wells:
 - Aquifers: detects in 30 (0.86%) of 3,496 samples at a median concentration of 0.085 µg/L.
 - Shallow ground water in urban areas: detects in 20 (2.4%) of 847 samples.
 - Shallow ground water in agricultural areas: detects in 1 (0.1%) of 723 samples.
 - Domestic wells: detects in 7 (0.29%) of 2,400 samples at a median concentration of 0.073 µg/L.
 - Public wells: detects in 22 (2.0%) of 1,096 samples at a median concentration of 0.22 µg/L.
 - Domestic and public wells: detects in 29 (0.8%) of 3,496 samples.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 1,423 (1.16%) of 123,019 drinking water samples; detects were from 35 (0.86%) of the 4,080 PWSs that reported data; detects ranged from 0.5 – 20.4 µg/L.
 - Illinois: not detected in 6 drinking water samples from 2 CWSs that reported data.
 - North Carolina: detects in 115 (0.58%) of 19,837 drinking water samples; detects were from 24 (0.96%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 8.8 µg/L.
 - Ohio: detects in 57 (0.61%) of 9,350 drinking water samples; detects were from 19 (0.75%) of the 2,537 PWSs that reported data; detects ranged from 0.5 – 5.32 µg/L.
 - Region 9 Tribes: not detected in 1,184 drinking water samples from 286 PWSs that reported data.
 - South Dakota: not detected in 1,110 drinking water samples from 281 PWSs that reported data.
 - Texas: detects in 12 (0.03%) of 36,287 drinking water samples; detects were from 5 (0.09%) of the 5,660 PWSs that reported data; detects ranged from 1.2 – 4.6 µg/L.
- *Florida Department of Environmental Protection (2004 – 2007)*: detects in 47 (2.66%) of the 1,766 drinking water samples; detects were from 4 (14.81%) of the 27 PWSs that reported data; detects ranged from 0.06 – 16.7 µg/L.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 228 (1.51%) of the 15,053 drinking water samples; detects were from 40 (2.07%) of the 1,930 PWSs that reported data; detects ranged from 0.061 – 15 µg/L.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 93 (1.44%) of the 6,472 drinking water samples; detects were from 9 (0.80%) of the 1,124 PWSs that reported data; detects ranged from 0.107 – 37 µg/L.
- *Community Water System Survey (CWSS) (2006)*: 1 system serving > 500,000 people reported monitoring data for 1,1-dichloroethane; system reported results of one sample only in which no 1,1-dichloroethane was detected.

Persistence & Mobility

- *Water Solubility*: 5,040 mg/L, indicates 1,1-dichloroethane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 35.04 L/kg, indicates 1,1-dichloroethane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 1.79, indicates 1,1-dichloroethane is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 5.62E-03 atm-m³/mol, indicates 1,1-dichloroethane is not very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 46% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 38 days, indicates 1,1-dichloroethane is moderately persistent in the environment.

References

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Grady, S.J. 2003. *A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4079, 85 p.

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UCMR 3 Analyte Information Sheet

Bromomethane (Methyl bromide)

CASRN: 74-83-9

Background & Use

- Bromomethane is a halogenated alkane and occurs as a gas. It is used as a fumigant on soil before planting, on crops after harvest, on vehicles and buildings, and for other specialized purposes.
- Office of Pesticide Programs (OPP) released a Tolerance Reassessment Progress and Risk Management Decision (RED) for bromomethane (under the name methyl bromide), and a Reregistration Eligibility Decision (RED) for commodity uses, in August of 2006. A RED for soil fumigant uses was released in July 2008 and amended in May 2009.
- Bromomethane is an ozone-destroying chemical regulated under the Montreal Protocol. Methyl bromide use in the U.S. was phased out in 2005, except for specific critical use exemptions and quarantine and preshipment exemptions. The most recent (2008) list of critical use exemptions includes a variety of applications to fruits and vegetables, nursery seedlings and ornamentals, plus several food processing and storage applications (72 FR 74118).
- Names & Synonyms: Bromomethane; methyl bromide; monobromomethane; methogas; brom-o-gas.
- Bromomethane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*:
 - 0.0014 mg/kg/day, based on a No Observed Adverse Effect Level (*No Observed Adverse Effect Level (NOAEL)*) of 1.4 mg/kg/day and an Uncertainty Factor (UF) of 1,000, and associated with epithelial hyperplasia in the forestomach (*Integrated Risk Information System [IRIS]*).
 - 0.001 mg/kg/day (*EPA Health Advisory [HA]*).
- *Minimal Risk Level (MRL)*: 0.003 mg/kg/day (*Agency for Toxic Substances and Disease Registry [ATSDR] Intermediate Minimal Risk Level (MRL)*).
- *NOAEL*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 29.9 mg/kg/day, based on a 2-year oral study in rats, and associated with changes in kidney, ureter, and bladder, and other changes in urine composition, changes in hair, and weight loss or decreased weight gain (*Registry of Toxic Effects of Chemical Substances [RTECS] Oral Chronic LOAEL*).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: 1 mg/kg/day (*Joint FAO/WHO Meeting on Pesticide Residues [JMPR] Maximum ADI*).

- *Cancer and/or Teratogen Class:*
 - D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
 - 3 – the agent is not classifiable as to its carcinogenicity to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Reproductive Effects*).
- *Drinking Water Equivalent Level (DWEL):* 0.05 mg/L.
- *Health Reference Level (HRL):* 9.8 µg/L for non-cancer effects in drinking water based on the IRIS RfD of 0.0014 mg/kg/day.

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR):* production was approximately > 10 – 50 million pounds in 1998 and > 1 – 10 million pounds in 2002.
- *OPP RED Estimated Usage:* approximately 12 million pounds active ingredient (a.i.) applied in 2007; as of January 2008, approximately 14 million pounds of pre-2005 stocks remained (after phase-out per the Montreal Protocol).
- *EPA Pesticide Industry Sales and Usage Report:* 28 – 33 million pounds a.i. used in the U.S. in 1999 and 20 – 25 million pounds a.i. used in the U.S. in 2001.
- *National Center for Food and Agricultural Policy (NCFAP) Pesticide Use Database:* approximately 33 million pounds a.i. used across 29 states in 1997.
- *United States Geological Survey (USGS) Pesticide Use Maps:* approximately 17.7 million pounds a.i. used in the U.S. in 2002.
- *Toxics Release Inventory (TRI) 2002:* facilities reported 112 pounds were released into surface water across 4 states, and a total of 539,555 pounds were released into the environment across 20 states.
- *TRI 2004:* facilities reported 200 pounds were released into surface water across 3 states, and a total of 552,208 pounds were released into the environment across 17 states.
- *TRI 2006:* facilities reported 361 pounds were released into surface water across 2 states, and a total of 408,252 pounds were released into the environment across 16 states.
- *High Production Volume (HPV) Challenge Program:* is included in the program which performs baseline testing on chemicals that are made or imported into the U.S. in amounts equal to or greater than one million pounds per year.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data:* analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 155 (0.77%) of the 20,198 PWSs, at a maximum concentration of 43 µg/L and a median concentration of 1 µg/L.
 - Round 2 (1993 – 1997): occurred at 175 (0.75%) of the 23,328 PWSs, at a maximum concentration of 38.1 µg/L and a median concentration of 1.6 µg/L.

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 81 (2.32%) of 3,486 samples; detects were from 70 (4.27%) of the 1,640 sites; detects were from 2 states; detects ranged from 0.2 – 50 µg/L.
 - Surface Water: detects in 514 (27.11%) of 1,896 samples; detects were from 84 (17.04%) of the 493 sites; detects were from 2 states; detects ranged from 0 – 2 µg/L.
 - Ohio Public Water Supply: not detected in 1,274 drinking water samples from 186 sites that reported data.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 3 (0.05%) of 5,952 samples and at 3 (0.069%) of the 4,317 sites at a maximum concentration of 0.5 µg/L and a median concentration of 0.1 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; detects in 2 (0.21%) of the samples (0.17% of ground water samples and 0.28% of surface water samples) at a concentration of 6.4 µg/L for ground water and 0.22 µg/L for surface water (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs. Below the reporting level of 0.2 µg/L, detected at 3.0% of the CWSs sampled (3.8% of ground water sites and 1.8% of surface water sites) at concentrations ranging from 0.09 – 0.11 µg/L (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 335 urban wells and 1,186 rural wells; 0% detection frequency in urban areas and 0.05% detection frequency in rural areas at a concentration of 0.05 µg/L (Squillace et al., 1999). (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
- *NAWQA VOCs in Ground Water and Drinking Water Supply Wells (1985 – 2001)*: national assessment comprised of approximately 100 different aquifer studies; roughly 3,500 water samples collected from various types of wells:
 - Aquifers: detects in 1 (0.032%) of 3,119 samples at a concentration of 0.50 µg/L.
 - Shallow ground water in urban areas: not detected in 847 samples.
 - Shallow ground water in agricultural areas: not detected in 723 samples.
 - Domestic wells: not detected in 2,156 samples.
 - Public wells: detects in 1 (0.093%) of 1,078 samples at a concentration of 6.4 µg/L.
 - Domestic and public wells: detects in 1 (< 0.1%) of 3,234 samples.

- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 72 (0.06%) of 112,570 drinking water samples; detects were from 51 (1.26%) of the 4,041 PWSs that reported data; detects ranged from 0.2 – 24 µg/L.
 - Illinois: not detected in 6 drinking water samples from 2 CWSs that reported data.
 - North Carolina: detects in 23 (0.12%) of 19,855 drinking water samples; detects were from 22 (0.88%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 23 µg/L.
 - Ohio: detects in 52 (0.56%) of 9,269 drinking water samples; detects were from 41 (1.62%) of the 2,531 PWSs that reported data; detects ranged from 0.5 – 24 µg/L.
 - Region 9 Tribes: detects in 1 (0.09%) of 1,163 drinking water samples at a concentration of 0.5 µg/L; 286 PWSs reported data.
 - South Dakota: not detected in 1,110 drinking water samples from 281 PWSs that reported data.
 - Texas: detects in 179 (0.49%) of 36,325 drinking water samples; detects were from 116 (2.05%) of the 5,660 PWSs that reported data; detects ranged from 0.51 – 65.54 µg/L.
- *Florida Department of Environmental Protection (2004 – 2007)*: detects in 1 (0.06%) of 1,767 drinking water samples at a concentration of 0.3 µg/L; 27 PWSs sampled.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 32 (0.21%) of 15,018 drinking water samples; detects were from 29 (1.50%) of the 1,929 PWSs that reported data; detects ranged from 0.06 – 3.5 µg/L.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 7 (0.11%) of 6,467 drinking water samples; detects were from 6 (0.53%) of the 1,123 PWSs that reported data; detects ranged from 0.19 – 1.6 µg/L.

Persistence & Mobility

- *Water Solubility*: 15,200 mg/L, indicates bromomethane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 9 – 22 L/kg, indicates bromomethane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 1.19, indicates bromomethane is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 0.00734 atm-m³/mol, indicates bromomethane is moderately mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 42% (*PBT Profiler*).
- *Estimated Biodegradation Half-Life*: 20 – 26.7 days, indicates bromomethane is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

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UCMR 3 Analyte Information Sheet

Chlorodifluoromethane (HCFC-22)

CASRN: 75-45-6

Background

- Chlorodifluoromethane is a chlorofluorocarbon and occurs as a gas. It is used as a refrigerant, as a low-temperature solvent, and in fluorocarbon resins, especially tetrafluoroethylene polymers.
- Names & Synonyms: Chlorodifluoromethane; HCFC-22; difluorochloromethane; monochlorodifluoromethane; fluorocarbon 22; freon 22.
- Chlorodifluoromethane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 13.5 mg/kg/day, based on a 26-week study in rats, and associated with degenerative effects on the brain and coverings; changes in the blood cell count (unspecified); and nutritional and gross metabolic effects, such as weight loss or decreased weight gain (*Registry of Toxic Effects of Chemical Substances [RTECS] Oral Chronic LOAEL*).
- *Hazardous Substances Data Bank (HSDB) Lowest Oral Lethal Dose (LD₅₀)*: 2,240 mg/kg.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - 3 – the agent is not classifiable as to its carcinogenicity to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 31.5 µg/L for non-cancer effects in drinking water based on the RTECS LOAEL of 13.5 mg/kg/day.

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 100 – 500 million pounds in 1998 and in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported that 2,632 pounds were released into surface water across 2 states, and a total of 9,229,794 pounds were released into the environment across 37 states.
- *TRI 2004*: facilities reported that 2,972 pounds were released into surface water in 1 state, and a total of 7,105,599 pounds were released into the environment across 35 states.

- *TRI 2006*: facilities reported that 2,798 pounds were released into surface water across 2 states, and a total of 7,017,573 pounds were released into the environment across 35 states.

Occurrence in Water

- No data for occurrence in water.

Persistence & Mobility

- *Water Solubility*: 2,770 mg/L, indicates chlorodifluoromethane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 35.04 L/kg, indicates chlorodifluoromethane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 1.08, indicates chlorodifluoromethane is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 0.0406 atm-m³/mol, indicates chlorodifluoromethane is not very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 43% (*PBT Profiler*).
- *Estimated Biodegradation Half-Life*: 15 days, indicates chlorodifluoromethane is moderately persistent in the environment.

UCMR 3 Analyte Information Sheet

Bromochloromethane (Halon 1011)

CASRN: 74-97-5

Background & Use

- Bromochloromethane is used as a fire-extinguishing fluid, an explosive suppressant, and as a solvent in the manufacturing of pesticides.
- Names & Synonyms: Bromochloromethane; Halon 1011; chlorobromomethane; methylene chlorobromide.
- Bromochloromethane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.01 mg/kg/day, associated with increased liver-to-body weight ratio and cloudy swelling and vacuolization of hepatocytes (*EPA Health Advisory [HA]*).
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
- *Drinking Water Equivalent Level (DWEL)*: 0.5 mg/L.
- *Health Reference Level (HRL)*: 70 µg/L for non-cancer effects in drinking water based on the EPA HA RfD of 0.01 mg/kg/day.

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 1 – 10 million pounds in 1998 and in 2002.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 65 (0.5%) of the 12,881 PWSs, at a maximum concentration of 210 µg/L and a median concentration of 1 µg/L.
 - Round 2 (1993 – 1997): occurred at 106 (0.46%) of the 22,974 PWSs, at a maximum concentration of 33.4 µg/L and a median concentration of 1 µg/L.

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 53 (3.30%) of 1,606 samples; detects were from 40 (6.28%) of the 637 sites; detects were from 2 states; detects ranged from 0.5 – 250 µg/L.
 - Surface Water: detects in 276 (41.82%) of 660 samples; detects were from 69 (37.70%) of the 183 sites; detects were from 2 states; detects ranged from 0.005 – 8 µg/L.
 - Ohio Public Water Supply: not detected in 1,277 drinking water samples from 186 sites that reported data.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 14 (0.24%) of 5,869 samples and at 7 (0.165%) of the 4,238 sites at a maximum concentration of 0.45 µg/L and a median concentration of 0.2 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 953 CWSs; not detected at the reporting level of 0.2 µg/L (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 3.7% of the CWSs sampled (5.1% of ground water sites and 1.8% of surface water sites) at concentrations ranging from 0.04 – 0.08 µg/L (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 180 urban wells and 1,241 rural wells; 1.11% detection frequency in urban areas and 0% detection frequency in rural areas; all detects in urban areas were at concentrations of 0.2 µg/L (Squillace et al., 1999) (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 40 (0.03%) of 117,632 drinking water samples; detects were from 19 (0.47%) of the 4,035 PWSs that reported data; detects ranged from 0.5 – 17 µg/L.
 - North Carolina: detects in 31 (0.16%) of 19,842 drinking water samples; detects were from 29 (1.16%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 48.46 µg/L.
 - Ohio: detects in 23 (0.25%) of 9,291 drinking water samples; detects were from 21 (0.83%) of the 2,533 PWSs that reported data; detects ranged from 0.5 – 12 µg/L.
 - South Dakota: detects in 1 (0.09%) of 1,110 drinking water samples at a concentration of 0.68 µg/L; 281 PWSs reported data.
 - Texas: detects in 5 (0.01%) of 36,284 drinking water samples; detects were from 5 (0.09%) of the 5,660 PWSs that reported data; detects ranged from 0.56 – 2.3 µg/L.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 2 (0.08%) of 2,468 drinking water samples; detects were from 2 (0.20%) of the 1,009 PWSs that reported data; detects ranged from 0.71 – 4.2 µg/L.

- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 1 (0.03%) of 3,420 drinking water samples at a concentration of 0.73 µg/L; 747 PWSs sampled.
- *American Water Works Association Research Foundation (AWWA) Research Foundation (AWWA)-EPA Study of Disinfection Byproducts (DBPs)*: not detected at any finished water sites sampled (Krasner et al., 2006).

Persistence & Mobility

- *Water Solubility*: 16,700 mg/L, indicates bromochloromethane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 24 L/kg, indicates bromochloromethane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 1.41, indicates bromochloromethane is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 0.00146 atm-m³/mol, indicates bromochloromethane is moderately mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 40% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 15 days, indicates bromochloromethane is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

Grady, S.J. 2003. *A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4079, 85 p.

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UCMR 3 Analyte Information Sheet

1,4-Dioxane

CASRN: 123-91-1

Background & Use

- 1,4-Dioxane is a cyclic aliphatic ether and is commonly used as a solvent or solvent stabilizer in the manufacture and processing of paper, cotton, textile products, automotive coolant, cosmetics, and shampoos.
- Names & Synonyms: 1,4-Dioxane; p-dioxane; 1,4-diethylene dioxide; di(ethylene oxide).
- 1,4-Dioxane is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.03 mg/kg/day, based on a No Observed Adverse Effect Level (*No Observed Adverse Effect Level (NOAEL)*) of 9.6 mg/kg/day in rats and an Uncertainty Factor (UF) of 300, and associated with liver and kidney toxicity (*Integrated Risk Information System [IRIS]*).
- *Minimal Risk Level (MRL)*:
 - 0.1 mg/kg/day (*Agency for Toxic Substances and Disease Registry [ATSDR]*).
 - 0.6 mg/kg/day (*ATSDR Intermediate Minimal Risk Level (MRL)*).
- *NOAEL*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*:
 - 0.011 (mg/kg/day)⁻¹ (*IRIS Oral Slope Factor*).
 - 0.19 (mg/kg/day)⁻¹ (*IRIS Draft Updated Oral Slope Factor, Draft Toxicological Review Released for External Review and Public Comment May 7, 2009; 74 FR 21361*).
 - 0.027 (mg/kg/day)⁻¹ (*California Office of Environmental Health and Hazard Assessment [OEHHA] Oral Slope Factor*).
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - B2 – probable human carcinogen (sufficient evidence from animal studies and inadequate/no epidemiologic studies) (*EPA Cancer Class*).
 - 2A – the agent is probably carcinogenic to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *EPA 10⁴ Lifetime Cancer Risk*: 0.3 mg/L.
- *Drinking Water Equivalent Level (DWEL)*: Not available.

- *Health Reference Level (HRL)*:
 - 700 µg/L for non-cancer effects in drinking water based on the ATSDR *Minimal Risk Level (MRL)* of 0.1 mg/kg/day.
 - 210 µg/L for non-cancer effects in drinking water based on the draft IRIS RfD of 0.03 mg/kg/day.
 - 30 µg/L for cancer effects in drinking water based on the EPA 10^{-4} lifetime cancer risk of 0.3 mg/L (*set at the 10^{-5} risk level*).
 - 1.84 µg/L for cancer effects in drinking water based on the draft IRIS oral slope factor of 0.19 mg/L (*set at the 10^{-5} risk level*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 1 – 10 million pounds in 1998 and in 2002.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 75,119 pounds released into surface water across 9 states, and a total of 1,146,641 pounds released into the environment across 22 states.
- *TRI 2004*: facilities reported 89,521 pounds were released into surface water across 7 states, and a total of 821,067 pounds were released into the environment across 22 states.
- *TRI 2006*: facilities reported 49,035 pounds were released into surface water across 8 states, and a total of 316,133 pounds were released into the environment across 19 states.

Occurrence in Water

- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review
 - California: detects in 505 (11.9%) of 4,245 drinking water samples; detects were from 24 (11.0%) of the 218 public water systems (PWSs) that reported data; detects ranged from 0.001 – 46.2 µg/L.
- *Community Water System Survey (CWSS) (2006)*: 1 system serving > 500,000 people reported monitoring data; detects in 17 (68%) of 25 samples; detects ranged from 0.5 – 2.2 µg/L.

Persistence & Mobility

- *Water Solubility*: 1,000,000 mg/L, indicates 1,4-dioxane is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 1 L/kg, indicates 1,4-dioxane is very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: -0.27, indicates 1,4-dioxane is very mobile in water.
- *Henry's Law Constant (K_{H1})*: 4.80E-06 atm-m³/mol, indicates 1,4-dioxane is moderately mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 47% (*PBT Profiler*).
- *Estimated Biodegradation Half-Life*: Not available.
- *Modeled or Measured Degradation Rates*: suggest that 1,4-dioxane is moderately persistent in the environment.

UCMR 3 Analyte Information Sheet

Vanadium

CASRN: 7440-62-2

Background & Use

- Vanadium is a naturally-occurring elemental metal. It is commonly used as vanadium pentoxide which is a chemical intermediate and a catalyst.
- Names & Synonyms: Vanadium.
- Vanadium is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.007 mg/kg/day (*Risk Assessment Information System [RAIS]*).
- *Minimal Risk Level (MRL)*: 0.003 mg/kg/day with an Uncertainty Factor (UF) of 100, and is associated with altered renal function indicated by increased plasma urea and mild histological changes (*Agency for Toxic Substances and Disease Registry [ATSDR] Intermediate Minimal Risk Level (MRL)*).
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 960 mg/kg/day, based on a study in domestic mammals (*Registry of Toxic Effects of Chemical Substances [RTECS]*).
- *RfD-Like Tolerable Upper Intake Level*: 0.026 mg/kg/day, associated with kidney lesions and increases in plasma urea and uric acid.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 21 µg/L for non-cancer effects in drinking water based on the ATSDR Intermediate Minimal Risk Level of 0.003 mg/kg/day.

Production & Release

- *Toxics Release Inventory (TRI) 2002*: facilities reported 2,666 pounds were released into surface water across 6 states, and a total of 2,417,562 pounds were released into the environment across 24 states.
- *TRI 2004*: facilities reported 1,170 pounds were released into surface water across 6 states, and a total of 1,600,795 pounds were released into the environment across 23 states.
- *TRI 2006*: facilities reported 16,889 pounds were released into surface water across 5 states, and a total of 2,591,471 pounds were released into the environment across 21 states.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 557 (19.29%) of 2,888 samples; detects were from 285 (42.73%) of the 667 sites; detects were from 10 states; detects ranged from 0.087 – 86,000 µg/L.
 - Surface Water: detects in 23,586 (54.46%) of 43,307 samples; detects were from 4,362 (43.59%) of the 10,006 sites; detects were from 33 states; detects ranged from 0 – 52,800 µg/L.
 - Ohio Public Water Supply: not detected in 1 drinking water sample from 1 site that reported data.
- *National Inorganics and Radionuclides Survey (NIRS) (1984 – 1986)*: detected at 146 (14.76%) of the 989 public water systems (PWSs) at a maximum concentration of 70 µg/L and a median concentration of 7 µg/L.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 16,688 (64.7%) of 25,784 drinking water samples; detects were from 1,824 (67.6%) of the 2,698 PWSs that reported data; detects ranged from 0.002 – 210 µg/L.
 - Illinois: not detected in 19 drinking water samples from 17 community water systems (CWSs) that reported data.
 - Ohio: not detected in 71 drinking water samples from 23 PWSs that reported data.

Persistence & Mobility

- *Water Solubility*: 8,000 mg/L, indicates vanadium pentoxide is highly mobile in the environment.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: Not available.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: Not available.
- *Estimated Biodegradation Half-Life*: Not available.
- *Modeled or Measured Degradation Rates*: suggest vanadium is highly persistent in the environment.

UCMR 3 Analyte Information Sheet

Molybdenum

CASRN: 7439-98-7

Background & Use

- Molybdenum is a naturally-occurring element found in ores and present in plants, animals, and bacteria. Its commonly used form, molybdenum trioxide, is used as a chemical reagent.
- Names & Synonyms: Molybdenum.
- Molybdenum is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.005 mg/kg/day, based on a Lowest Observed Adverse Effect Level (LOAEL) of 0.14 mg/kg/day and an Uncertainty Factor (UF) of 30, and associated with increased uric acid levels. (*Integrated Risk Information System [IRIS]*).
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *LOAEL*: 0.5 mg/kg/day, based on a 19-week study in rabbits, and associated with effects on the liver, kidneys, ureter, and the bladder, and effects on nutritional and gross metabolic conditions, such as weight loss or decreased weight gain (*Registry of Toxic Effects of Chemical Substances [RTECS]*).
- *Institute of Medicine (IOM) Tolerable Upper Intake Level*: 0.03 mg/kg/day, associated with effects on reproduction and fetal development (decreased gestational weight gain, prolonged estrus cycle, and failure to breed), renal failure, diuresis, and proteinuria.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
 - Listed (*University of Maryland's Partial List of Teratogens*).
- *Drinking Water Equivalent Level (DWEL)*: 0.2 mg/L.
- *Health Reference Level (HRL)*: 35 µg/L for non-cancer effects in drinking water based on the IRIS RfD of 0.005 mg/kg/day.

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: no reports for 1998 or 2002; however, production was approximately > 1 million - 10 million pounds in 1986.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 388 (24.89%) of 1,559 samples; detects were from 170 (34.69%) of the 490 sites; detects were from 9 states; detects ranged from 0 – 4,000 µg/L.
 - Surface Water: detects in 18,231 (45.71%) of 39,884 samples; detects were from 3,854 (37.37%) of the 10,313 sites; detects were from 28 states; detects ranged from 0 – 75,000 µg/L.
- *National Inorganics and Radionuclides Survey (NIRS) (1984 – 1986)*: detected at 77 (7.79%) of the 989 public water systems (PWSs) at a maximum concentration of 181 µg/L and a median concentration of 10 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 2,927 (52%) of 5,628 samples and at 1,879 (57%) of the 3,297 sites at a maximum concentration of 4,732.80 µg/L and a median concentration of 3 µg/L.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 1,132 (49.50%) of 2,287 drinking water samples; detects were from 107 (66.46%) of the 161 PWSs that reported data; detects ranged from 0.005 – 83 µg/L.
 - Illinois: detects in 252 (13.19%) of 1,911 drinking water samples; detects were from 149 (17.23%) of the 865 community water systems (CWSs) that reported data; detects ranged from 2.5 – 110 µg/L.
 - Ohio: detects in 34 (44.74%) of 76 drinking water samples; detects were from 13 (50.0%) of the 26 PWSs that reported data; detects ranged from 1 – 64 µg/L.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: not detected in 2 drinking water samples from 1 PWS that reported data.

Persistence & Mobility

- *Water Solubility*: 1,066 mg/L, indicates molybdenum trioxide is highly mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: Not available.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: Not available.
- *Estimated Biodegradation Half-Life*: Not available.
- *Modeled or Measured Degradation Rates*: suggest molybdenum is highly persistent in the environment.

UCMR 3 Analyte Information Sheet

Cobalt

CASRN: 7440-48-4

Background & Use

- Cobalt is a naturally-occurring element found in the earth's crust, and at low concentrations in seawater and in some surface and ground water. Cobalt chloride was formerly used in medicine and as a germicide.
- Names & Synonyms: Cobalt.
- Cobalt is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.02 mg/kg/day (*Risk Assessment Information System [RAIS]*).
- *Minimal Risk Level (MRL)*: 0.01 mg/kg/day with an Uncertainty Factor (UF) of 100, and associated with blood increased hemoglobin, polycythemia, and respiratory-effects on lung function (*Agency for Toxic Substances and Disease Registry [ATSDR] Intermediate Minimal Risk Level (MRL)*).
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *International Toxicity Estimates for Risk (ITER) Tolerable Daily Intake (TDI)*: 0.0014 mg/kg/day, based on a Lowest Observed Adverse Effect Level (LOAEL) of 0.04 mg/kg/day and an UF of 30, and associated with heart effects.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - 2B – the agent is possibly carcinogenic to humans (*International Agency for Research on Cancer [IARC] Cancer Class*).
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 70 µg/L for non-cancer effects in drinking water based on the ATSDR Intermediate Minimal Risk Level of 0.01 mg/kg/day.
- *CDC's 95th Percentile Concentration*: 1.32 µg/L for 2,465 urine samples tested from 1999 – 2000; 1.28 µg/L for 2,690 urine samples tested from 2001 – 2002; and 1.16 µg/L for 2,558 urine samples tested from 2003 – 2004 (*Calafat et al., 2007*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: no reports for 1998 or 2002; however, production was approximately > 10,000 - 500,000 pounds in 1986 and in 1990.

- *Toxics Release Inventory (TRI) 2002*: facilities reported 2,784 pounds were released into surface water across 19 states, and a total of 748,062 pounds were released into the environment across 38 states.
- *TRI 2004*: facilities reported 1,227 pounds were released into surface water across 17 states, and a total of 776,762 pounds were released into the environment across 38 states.
- *TRI 2006*: facilities reported 760 pounds were released into surface water across 18 states, and a total of 943,396 pounds were released into the environment across 37 states.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 467 (19.12%) of 2,442 samples; detects were from 197 (28.14%) of the 700 sites; detects were from 9 states; detects ranged from 0 – 21,100 µg/L.
 - Surface Water: detects in 13,254 (24.00%) of 55,217 samples; detects were from 4,855 (40.88%) of the 11,877 sites; detects were from 30 states; detects ranged from 0 – 245,800 µg/L.
- *National Inorganics and Radionuclides Survey (NIRS) (1984 – 1986)*: detected at 3 (0.30%) of the 989 of public water systems (PWSs) at a maximum concentration of 11 µg/L and a median concentration of 10 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 1,170 (20.78%) of 5,630 samples and at 782 (23.7%) of the 3,297 sites at a maximum concentration of 684 µg/L, and a median concentration of 0.22 µg/L.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 74 (3.27%) of 2,266 drinking water samples; detects were from 10 (14.93%) of the 67 PWSs that reported data; detects ranged from 0.01 – 10 µg/L.
 - Illinois: detects in 1 (3.85%) of 26 drinking water samples at a concentration of 11 µg/L; 22 community water systems (CWSs) reported data.
 - Ohio: detects in 3 (4.11%) of 73 drinking water samples; detects were from 3 (12.0%) of the 25 PWSs that reported data; detects ranged from 3.36 – 10 µg/L.

Persistence & Mobility

- *Water Solubility*: 1,160,000 mg/L, indicates cobaltous chloride is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: Not available.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: Not available.
- *Estimated Biodegradation Half-Life*: Not available.
- *Modeled or Measured Degradation Rates*: suggest cobalt is persistent in the environment.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

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UCMR 3 Analyte Information Sheet

Strontium

CASRN: 7440-24-6

Background & Use

- Strontium is a naturally-occurring element. Historically, the commercial use of strontium has been in the faceplate glass of cathode-ray tube televisions, to block x-ray emissions.
- Names & Synonyms: Strontium.
- Strontium is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.6 mg/kg/day, based on a No Observed Adverse Effect Level (NOAEL) of 190 mg/kg/day in rats and an Uncertainty Factor (UF) of 300, and associated with rachitic bone (*Integrated Risk Information System [IRIS]*).
- *Minimal Risk Level (MRL)*: 2 mg/kg/day with an UF of 30, and is associated with musculoskeletal effects (*Agency for Toxic Substances and Disease Registry [ATSDR] Intermediate Minimal Risk Level (MRL)*).
- *NOAEL*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
- *Drinking Water Equivalent Level (DWEL)*: 20 mg/L.
- *Health Reference Level (HRL)*: 4,200 µg/L for non-cancer effects in drinking water based on the IRIS RfD of 0.6 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 1,778 (94.98%) of 1,872 samples; detects were from 707 (96.19%) of the 735 sites; detects were from 14 states; detects ranged from 0 – 19,000 µg/L.
 - Surface Water: detects in 24,059 (93.77%) of 25,657 samples; detects were from 7,999 (98.15%) of the 8,150 sites; detects were from 27 states; detects ranged from 0.01 – 19,034,000 µg/L.

- Ohio Public Water Supply: detects in 3,070 (99.42%) of 3,088 samples; detects were from 187 (100%) of the 187 sites; detects were from 1 (100%) state; detects ranged from 52 – 66,200 µg/L.
- *National Water-Quality Assessment (NAWQA) U.S. Domestic Wells (1991 – 2004)*: detects in 485 (99.4%) of 488 well samples from aquifer studies; detects in 82 (100%) of 82 samples from agricultural land-use studies (DeSimone, 2009).
- *Contaminants in Ground Water of the Glacial Aquifer System in the Northern U.S. (1991 – 2003)*: detects in 551 (99.8%) of 552 samples analyzed; detects ranged from 1.47 – 9,120 µg/L (Groschen et al., 2008).
- *National Inorganics and Radionuclides Survey (NIRS) (1984 – 1986)*: detected at 980 (99.09%) of the 989 public water systems (PWSs) at a maximum concentration of 43.55 mg/L and a median concentration of 0.18 mg/L.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review
 - Illinois: detects in 21 (100%) of 21 drinking water samples; detects were from 19 (100%) of the 19 community water systems (CWSs) that reported data; detects ranged from 71 – 4,600 µg/L.
 - Ohio: detects in 75 (97.40%) of 77 drinking water samples; detects were from 30 (93.75%) of the 32 PWSs that reported data; detects ranged from 4 – 40,889 µg/L.
 - Region 9 Tribes: not detected in 1 drinking water sample from 1 PWS that reported data.
- *Community Water System Survey (CWSS) (2006)*: detected at 1 (1%) of the 94 systems serving more than 500,000 people, with a concentration of 330 µg/L.
- *Environmental Working Group (EWG) National Drinking Water Database (2004 – 2009)*: detected at 366 PWSs in 5 states (Wisconsin, Illinois, Ohio, New York, and Minnesota) (EWG, 2009.).

Persistence & Mobility

- *Water Solubility*: 11 mg/L, indicates strontium carbonate is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: Not available.
- *Henry's Law Constant (K_{H})*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System (W^0)*: Not available.
- *Estimated Biodegradation Half-Life*: Not available.

References

DeSimone, L.A. (2009). *Quality of water from domestic wells in principal aquifers of the United States, 1991-2004*. U. S. Geological Survey Scientific Investigations Report 2008-5227, 139 p. Available online at <http://pubs.usgs.gov/sir/2008/5227/>. Retrieved July 28, 2009.

EWG. 2009. National Drinking Water Database. Available on the Internet at: <http://www.ewg.org/tap-water/home>.

Groschen, G.E., T.L. Arnold, W.S. Morrow, and K.L. Warner. 2008. *Occurrence and distribution of iron, manganese, and selected trace elements in ground water in the glacial aquifer system of the Northern United States*. U.S. Geological Survey Scientific Investigations Report 2009–5006, 89 p. Available online at <http://pubs.usgs.gov/sir/2009/5006/>. Accessed January 21, 2010.

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UCMR 3 Analyte Information Sheet

Chlorate

CASRN: 14866-68-3

Several data points in this information sheet relate to sodium chlorate, as noted.

Background & Use

- Chlorate is an agricultural defoliant or desiccant, is a disinfectant byproduct and is used in the production of chlorine dioxide.
- Office of Pesticide Programs (OPP) released a Reregistration Eligibility Decision (RED) for inorganic chlorates in July of 2006.
- Names & Synonyms: Chlorate.
- Chlorate is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: 0.03 mg/kg/day, associated with thyroid hypertrophy and mineralization (OPP).
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Effect Level (NOEL)*: 5 mg/kg/day for sodium chlorate, associated with bone marrow hyperplasia, thyroid follicular hypertrophy, and mineralization (*National Toxicology Program [NTP] Supplemental NOEL*).
- *Lowest Observed Adverse Effect Level (LOAEL)*: 1.4 mg/kg/day for sodium chlorate, based on a 1-year study in rats (*Registry of Toxic Effects of Chemical Substances [RTECS] Oral Chronic LOAEL*).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 210 µg/L for non-cancer effects in drinking water based on the OPP RfD of 0.03 mg/kg/day.

Production & Release

- *OPP RED Estimated Usage*: approximately 2.8 million pounds active ingredient (a.i.) of sodium chlorate used annually in the U.S. (no data range provided).
- *National Center for Food and Agricultural Policy (NCFAP) Pesticide Use Database*: approximately 7 million pounds a.i. of sodium chlorate used across 16 states in 1997.
- *United States Geological Survey (USGS) Pesticide Use Maps*: approximately 4.8 million pounds a.i. used in the U.S. in 2002.

Occurrence in Water

- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 945 (78.4%) of 1,205 drinking water samples; detects were from 24 (53.3%) of the 45 public water systems (PWSs) that reported data; detects ranged from 0.01 to 747 µg/L.
- *Disinfection By-Product Information Collection Rule (DBP-ICR) (1997 – 1998)*: detects in 1,490 (86.7%) of 1,719 samples at a maximum concentration of 2,234 µg/L and a median concentration of 120 µg/L.
- *Community Water System Survey (CWSS) (2006)*: detects in 2 (50%) of 4 samples, at concentrations of 34 and 51 µg/L.
- *Fourteen U.S. Drinking Water Utilities*: detects in 2 (14%) of 14 source water samples, at concentrations of 20 and 22 µg/L; detects in 14 (100%) of 14 samples disinfected with hypochlorite solution at concentrations ranging from 11 – 660 µg/L; detects in 14 (100%) of 14 hypochlorite solutions, at concentrations ranging from 0.18 – 42 g/L; second set of analyses performed on the same solutions approximately four months later - detects in 14 (100%) of 14 solutions, at concentrations ranging from 0.19 – 50 g/L (Bolyard et al., 1992).
- *Forty-Two U.S. Drinking Water Utilities* (follow-up study to Bolyard et al., 1992): detects in 2 (13%) of 15 source water samples, at concentrations of 19 and 23 µg/L in utilities that use hypochlorite solution disinfection; detects in 16 (100%) of 16 drinking water samples at concentrations ranging from 11 – 660 µg/L in utilities that use hypochlorite solution disinfection; detects in 2 (12.5%) of 16 source water samples at concentrations of 17 and 81 µg/L in utilities that use gaseous chlorine disinfection; detects in 3 (11%) of 28 drinking water samples at concentrations ranging from 17 – 43 µg/L in utilities that use gaseous chlorine disinfection (Bolyard et al., 1993).

Persistence & Mobility

- *Water Solubility*: 1,000,000 mg/L for sodium chlorate, indicates sodium chlorate is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: Not available.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: Not available.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System (W^0)*: Not available.
- *Estimated Biodegradation Half-Life*: Not available.

References

Bolyard, M., P.S. Fair, and D.P. Hautman. 1992. Occurrence of chlorate in hypochlorite solutions used for drinking water disinfection. *Environmental Science and Technology*. 26(8): 1663-1665.

Bolyard, M., P.S. Fair, and D.P. Hautman. 1993. Sources of chlorate ion in U.S. drinking water. *Journal of American Water Works Association*. 85(9): 81-88.

UCMR 3 Analyte Information Sheet

Perfluorooctanesulfonic Acid (PFOS)

CASRN: 1763-23-1

Background & Use

- Perfluorooctanesulfonic acid (PFOS) is used as a surfactant or emulsifier in fire fighting foam, circuit board etching acids, alkaline cleaners, and floor polish, and as a pesticide active ingredient for insect bait traps. The sole U.S. manufacturer of PFOS phased out production of the chemical in 2002. However, PFOS is still generated incidentally.
- Names & Synonyms: Perfluorooctanesulfonic acid; PFOS; perfluorooctane sulfonate; heptadecafluorooctane-1-sulphonic acid; perfluorooctylsulfonic acid.
- PFOS is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*:
 - 0.03 mg/kg/day associated with decreased body weights, increased liver weights, lowered serum total cholesterol, lowered triiodothyronine (T3) concentration, and lowered estradiol levels (*EPA Provisional Health Advisory [HA]*).
 - 0.1 mg/kg/day, based on a 2 generation reproductive study in rats, and associated with reduced F2 body weight (*65 FR 62319*).
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Hazardous Substances Data Bank (HSDB) Lowest Oral Lethal Dose (LD₅₀)*: 251 mg/kg.
- *EPA Provisional HA*: 0.2 µg/L.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *EPA Provisional HA*: 0.2 µg/L.
- *Health Reference Level (HRL)*: 0.2 µg/L for non-cancer effects in drinking water based on the provisional HA NOAEL of 0.03 mg/kg/day.
- *CDCs 95th Percentile Concentration*: 54.6 µg/L for 2,094 serum samples tested from 2003 – 2004; detects in 99.9% of samples (*Calafat et al., 2007*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 10,000 – 500,000 pounds in 2002.

Occurrence in Water

- *New Jersey Department of Environmental Protection, Division of Water Supply (2007)*: detected at 13 (57%) of the 23 sites sampled at concentrations ranging from 0.0042 – 0.019 µg/L.
- *Minnesota Wells*: detected at 6 (16.2%) of the 37 municipal wells sampled at a maximum concentration of 1.4 µg/L; not detected at the 26 private wells sampled; not detected at the 22 non-community wells sampled (Goeden and Kelly, 2006).
- *Minnesota's Ambient Environment (2006 – 2008) (Minnesota Pollution Control Agency, 2008)*:
 - Rural Ambient Shallow Ground Water (October 2007): not detected in 22 samples.
 - Urban Ambient Shallow Ground Water (2006 – 2007): detects in 10 (34%) of 29 samples at a maximum concentration of 0.037 µg/L and a median concentration of 0.0105 µg/L.
 - Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 3 (9%) of 34 samples at a maximum concentration of 0.0582 µg/L and a median concentration of 0.00523 µg/L (includes estimated values).
 - Mississippi and Minnesota River Water Samples (August 2008): detects in 8 (23%) of 35 samples at a maximum concentration of 0.17 µg/L and a median concentration of 0.0124 µg/L.
 - Surface Water Samples (2006): detects in 6 (38%) of 16 samples at a maximum concentration of 0.115 µg/L and a median concentration of 0.0709 µg/L.
 - Brainerd Area Mississippi River Surface Water Samples (2007): detects in 2 (25%) of 8 samples at concentrations of 0.0936 and 0.102 µg/L.
 - Mississippi River Surface Water Samples (June 2008): detects in 9 (41%) of 22 samples at a maximum concentration of 0.00695 µg/L and a median concentration of 0.00598 µg/L.
 - City Road Drainage Ditch Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.140 µg/L and a median concentration of 0.132 µg/L.
 - Rice Lake Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.122 µg/L and a median concentration of 0.110 µg/L.

Persistence & Mobility

- *Water Solubility*: 370 mg/L (potassium salt of PFOS), indicates PFOS is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 100,000 L/kg, indicates PFOS is not very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 0.94, indicates PFOS is very mobile in water.
- *Henry's Law Constant (K_H)*: Not available.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 1% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: Not available.

- *Modeled or Measured Degradation Rates*: suggest that PFOS is persistent in the environment.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

Goeden, H. and J. Kelly. 2006. *Targeted Sampling 2004 – 2005*. Perfluorochemicals in Minnesota, MN DOH, 2/27/06.

Minnesota Pollution Control Agency. 2008. *PFCs in Minnesota's Ambient Environment*. 2008 Progress Report.

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UCMR 3 Analyte Information Sheet

Perfluorooctanoic Acid (PFOA)

CASRN: 335-67-1

Background & Use

- Perfluorooctanoic acid (PFOA) is a perfluorinated aliphatic carboxylic acid, commonly used for its emulsifier and surfactants properties in or as fluoropolymers (such as Teflon), fire-fighting foams, cleaners, cosmetics, greases and lubricants, paints, polishes, adhesives, and photographic films.
- Names & Synonyms: Perfluorooctanoic acid; PFOA; octanoic acid, pentadecafluoro-.
- PFOA is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 0.46 mg/kg/day, associated with body weight reduction, and increased liver, kidney, and brain weight relative to body weight (*Lau et al., 2006*).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 1.1 µg/L for non-cancer effects in drinking water based on the LOAEL of 0.46 mg/kg/day.
- *CDC's 95th Percentile Concentration*: 9.8 µg/L for 2,094 serum samples tested from 2003 – 2004; detects in 99.7% of samples (*Calafat et al., 2007*).

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 10,000 – 500,000 pounds in 1998 and in 2002.

Occurrence in Water

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 334 (47.71%) of 700 samples; detects were from 84 (87.50%) of the 96 sites; detects were from 1 state; detects ranged from 0.025 – 48,500 µg/L.
 - Surface Water: detects in 289 (49.57%) of 583 samples; detects were from 51 (63.75%) of the 80 sites; detects were from 1 state; detects ranged from 0.025 – 794 µg/L.

- *New Jersey Department of Environmental Protection, Division of Water Supply (2007)*: detected at 18 (78%) of the 23 sites sampled at concentrations ranging from 0.0045 – 0.039 µg/L.
- *Minnesota Wells*: detected at 6 (16.2%) of the 37 municipal wells sampled at a maximum concentration of 0.9 µg/L; detected at 1 (3.8%) of the 26 private wells sampled at a concentration of 0.67 µg/L; not detected at the 22 non-community wells sampled (Goeden and Kelly, 2006).
- *Testing of the Municipal Water System of Little Hocking, OH (2002 – 2005)*: concentrations in the water distribution system ranged from 1.5 – 7.2 µg/L, with a mean value of 3.55 µg/L; private wells in the area exhibited concentrations that ranged from < 0.01 – 14 µg/L (Emmett et al., 2006).
- *Minnesota's Ambient Environment (2006 – 2008) (Minnesota Pollution Control Agency, 2008)*:
 - Rural Ambient Shallow Ground Water (October 2007): not detected in 22 samples.
 - Urban Ambient Shallow Ground Water (2006 – 2007): detects in 4 (12%) of 29 samples at a maximum concentration of 0.0275 µg/L and a median concentration of 0.00871 µg/L.
 - Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 4 (12%) of 34 samples at a maximum concentration of 0.0364 µg/L and a median concentration of 0.003275 µg/L (includes estimated values).
 - Mississippi and Minnesota River Water Samples (August 2008): detects in 15 (43%) of 35 samples at a maximum concentration of 0.0196 µg/L and a median concentration of 0.00719 µg/L.
 - Surface Water Samples (2006): detects in 11 (69%) of 16 samples at a maximum concentration of 0.0325 µg/L and a median concentration of 0.0181 µg/L.
 - Brainerd Area Mississippi River Surface Water Samples (2007): detects in 2 (25%) of 8 samples at concentrations of 0.00499 and 0.00567 µg/L.
 - Mississippi River Surface Water Samples (June 2008): detects in 20 (91%) of 22 samples at a maximum concentration of 0.011 µg/L and a median concentration of 0.00468 µg/L.
 - City Road Drainage Ditch Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.059 µg/L and a median concentration of 0.0565 µg/L.
 - Rice Lake Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.042 µg/L and a median concentration of 0.0388 µg/L.

Persistence & Mobility

- *Water Solubility*: 9,500 mg/L, indicates PFOA is very mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 27,000 L/kg, indicates PFOA is not very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 2.68, indicates PFOA is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 0.091 atm-m³/mol, indicates PFOA is not very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 1% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 180 days, indicates PFOA is persistent in the environment.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

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UCMR 3 Analyte Information Sheet

Perfluorononanoic Acid (PFNA)

CASRN: 375-95-1

Background & Use

- Perfluorononanoic acid is a manmade chemical and is used in products to make them stain, grease, heat, and water resistant.
- Names & Synonyms: Perfluorononanoic acid; PFNA; perfluoro-n-nonanoic acid.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*:
 - 54 mg/kg/day, associated with death of all 10 mice before day 14 (*Kennedy, 1987*).
 - 0.5 mg/kg/day, based on a 21 day mouse dietary study, associated with hepatic effects (*Kennedy, 1987*).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 3.5 µg/L for non-cancer effects in drinking water based on the LOAEL of 0.5 mg/kg/day.
- *CDC's 95th Percentile Concentration*: 3.2 µg/L for 2,094 serum samples tested from 2003 – 2004; detects in 98.8% of samples (*Calafat et al., 2007*).

Production & Release

- No data for production and release.

Occurrence in Water

- *U.S. Drinking Water Utilities (2007)*: Seven U.S. drinking water utilities with increasing impacts of treated wastewater; planned indirect potable reuse facilities (2) were excluded (*Quiñones and Snyder, 2009*):
 - Utility 1: not detected in raw or finished samples.
 - Utility 2: detects in 4 (67%) of 6 raw samples at an average concentration of 0.0013 µg/L and detects in 5 (83%) of 6 finished samples at an average concentration of 0.0013 µg/L.
 - Utility 3: not detected in raw samples and detects in 1 (3%) of 33 finished samples at a concentration of 0.0010 µg/L.

- Utility 4: not detected in raw or finished samples.
- Utility 5: detects in 5 (100%) of 5 raw samples at an average concentration of 0.010 µg/L and detects in 7 (100%) of 7 finished samples at an average concentration of 0.0097 µg/L.
- *Minnesota's Ambient Environment (2006 – 2008) (Minnesota Pollution Control Agency, 2008):*
 - Rural Ambient Shallow Ground Water (October 2007): not detected in 22 samples.
 - Urban Ambient Shallow Ground Water (2006 – 2007): detects in 1 (3%) of 29 samples at a concentration of 0.00121 µg/L (a concentration less than the reporting level of 0.0025 µg/L).
 - Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 1 (3%) of 34 samples at a concentration of 0.00318 µg/L (estimated value).
 - Mississippi and Minnesota River Water Samples (August 2008): detects in 9 (26%) of 35 samples at a maximum concentration of 0.00719 µg/L and a median concentration of 0.00392 µg/L.
 - Surface Water Samples (2006): detects in 1 (6%) of 16 samples at a concentration of 0.00132 µg/L.
 - Brainerd Area Mississippi River Surface Water Samples (2007): detects in 2 (25%) of 8 samples at concentrations of 0.00258 and 0.00307 µg/L.
 - Mississippi River Surface Water Samples (June 2008): not detected in 22 samples.
 - City Road Drainage Ditch Surface Water Samples (2008): detects in 1 (33%) of 3 samples at a concentration of 0.00306 µg/L.
 - Rice Lake Surface Water Samples (2008): not detected in 3 samples.
- *Albany, New York Rain, Snow, Surface Runoff, and Lake Samples (2006 – 2007):* concentrations from 11 lake water samples ranged from not detected – 0.00351 µg/L with a median concentration of 0.00163 µg/L; concentrations from 11 rain water samples ranged from less than the Limit of Quantitation (LOQ) – 0.00348 µg/L with a median concentration of 0.00104 µg/L; concentrations from 21 snow samples ranged from < LOQ – 0.00494 µg/L with a median concentration of 0.00055 µg/L; concentrations from 14 surface runoff samples ranged from < LOQ – 0.00590 µg/L with a median concentration of 0.00071 µg/L (Kim and Kannan, 2007).
- *Cape Fear Drainage Basin in North Carolina (2006):* 100 water samples were collected from 80 different sites; detected above the LOQ (0.001 µg/L) in 74.7% of the samples; a maximum concentration of 0.194 µg/L and a median concentration of 0.0057 µg/L (Nakayama et al., 2007).

Persistence & Mobility

- No data for persistence and mobility.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11):1578-1583.

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Quiñones, O. and S.A. Snyder. 2009. Occurrence of perfluoroalkyl carboxylates and sulfonates in drinking water utilities and related waters from the United States. *Environmental Science and Technology*. 43: 9089-9095.

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UCMR 3 Analyte Information Sheet

Perfluorohexanesulfonic Acid (PFHxS)

CASRN: 355-46-4

Background & Use

- Perfluorohexanesulfonic acid is a manmade chemical and is used in products to make them stain, grease, heat, and water resistant.
- Names & Synonyms: Perfluorohexanesulfonic acid; PFHxS; perfluorohexane sulfonate; perfluorohexane-1-sulphonic acid.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: 10 mg/kg/day, based on a 42 – 56 day Sprague-Dawley rat study, associated with immuno/lymphoret, neurological, reproductive, and developmental effects (*Hoberman and York, 2003*).
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 70 µg/L for non-cancer effects in drinking water based on the NOAEL of 10 mg/kg/day.
- *CDC's 95th Percentile Concentration*: 8.3 µg/L for 2,094 serum samples tested from 2003 – 2004; detects in 98.3% of samples (*Calafat et al., 2007*).

Production & Release

- No data for production and release.

Occurrence in Water

- *U.S. Drinking Water Utilities (2007)*: Seven U.S. drinking water utilities with increasing impacts of treated wastewater; planned indirect potable reuse facilities (2) were excluded (Quiñones and Snyder, 2009):
 - Utility 1: not detected in raw or finished samples.
 - Utility 2: detects in 5 (83%) of 6 raw samples at an average concentration of 0.0021 µg/L and detects in 6 (100%) of 6 finished samples at an average concentration of 0.0022 µg/L.
 - Utility 3: not detected in raw or finished samples.

- Utility 4: detects in 2 (33%) of 6 raw samples at an average concentration of 0.0025 µg/L and detects in 3 (43%) of 7 finished samples at an average concentration of 0.0014 µg/L.
- Utility 5: detects in 5 (100%) of 5 raw samples at an average concentration of 0.012 µg/L and detects in 7 (100%) of 7 finished samples at an average concentration of 0.012 µg/L.
- *Minnesota's Ambient Environment (2006 – 2008) (Minnesota Pollution Control Agency, 2008):*
 - Rural Ambient Shallow Ground Water (October 2007): not detected in 22 samples.
 - Urban Ambient Shallow Ground Water (2006 – 2007): detects in 11 (38%) of 29 samples at a maximum concentration of 0.0778 µg/L and a median concentration of 0.00746 µg/L (includes concentrations less than the reporting level of 0.0025 µg/L).
 - Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 1 (3%) of 34 samples at a concentration of 0.168 µg/L (estimated value).
 - Mississippi and Minnesota River Water Samples (August 2008): detects in 2 (6%) of 35 samples at concentrations of 0.00936 and 0.00987 µg/L.
 - Surface Water Samples (2006): detects in 3 (19%) of 16 samples at a maximum concentration of 0.0271 µg/L and a median concentration of 0.0265 µg/L.
 - Brainerd Area Mississippi River Surface Water Samples (2007): not detected in 8 samples.
 - Mississippi River Surface Water Samples (June 2008): detects in 5 (23%) of 22 samples at a maximum concentration of 0.0066 µg/L and a median concentration of 0.00555 µg/L.
 - City Road Drainage Ditch Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.384 µg/L and a median concentration of 0.363 µg/L.
 - Rice Lake Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.255 µg/L and a median concentration of 0.253 µg/L.
- *Albany, New York Rain, Snow, Surface Runoff, and Lake Samples (2006 – 2007):* concentrations from 11 lake water samples ranged from less than the Limit of Quantitation (LOQ) – 0.00405 µg/L with a median concentration of 0.00053 µg/L; concentrations from 11 rain water samples ranged from not detected – 0.00036 µg/L with a median concentration of < LOQ; concentrations from 21 snow samples ranged from not detected – 0.00035 µg/L with a median concentration of < LOQ; concentrations from 14 surface runoff samples ranged from not detected – 0.0135 µg/L with a median concentration of 0.00035 µg/L (Kim and Kannan, 2007).
- *Cape Fear Drainage Basin in North Carolina (2006):* 100 water samples were collected from 80 different sites; detected above the LOQ (0.001 µg/L) in 73.4% of the samples; a maximum concentration of 0.0351 µg/L and a median concentration of 0.00566 µg/L (Nakayama et al., 2007).

Persistence & Mobility

- No data for persistence and mobility.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

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Kim, S-K. and K. Kannan. 2007. Perfluorinated acids in air, rain, snow, surface runoff, and lakes: Relative importance of pathways to contamination of urban lakes. *Environmental Science and Technology*. 41: 8328-8334.

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UCMR 3 Analyte Information Sheet

Perfluoroheptanoic Acid (PFHpA)

CASRN: 375-85-9

Background & Use

- Perfluoroheptanoic acid is a manmade chemical and is used in products to make them stain, grease, heat, and water resistant.
- Names & Synonyms: Perfluoroheptanoic acid; PFHpA; perfluoro-n-heptanoic acid; tridecafluoroheptanoic acid.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: Not available.
- *CDC's 95th Percentile Concentration*: 0.400 µg/L for 2,094 serum samples tested from 2003 – 2004; detects in 6.2% of samples (*Calafat et al., 2007*); no drinking water and/or toxicological data are currently available.

Production & Release

- No data for production and release.

Occurrence in Water

- *Minnesota's Ambient Environment (2006 – 2008) (Minnesota Pollution Control Agency, 2008)*:
 - Rural Ambient Shallow Ground Water (October 2007): not detected in 22 samples.
 - Urban Ambient Shallow Ground Water (2006 – 2007): detects in 13 (45%) of 29 samples at a maximum concentration of 0.0151 µg/L and a median concentration of 0.0037 µg/L (includes concentrations less than the reporting level of 0.0025 µg/L).
 - Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 1 (3%) of 34 samples at a concentration of 0.0162 µg/L (estimated value).
 - Mississippi and Minnesota River Water Samples (August 2008): detects in 8 (23%) of 35 samples at a maximum concentration of 0.00442 µg/L and a median concentration of 0.00384 µg/L (concentrations include estimated values).

- Surface Water Samples (2006): detects in 7 (44%) of 16 samples at a maximum concentration of 0.00476 µg/L and a median concentration of 0.00357 µg/L.
- Brainerd Area Mississippi River Surface Water Samples (2007): not detected in 8 samples.
- Mississippi River Surface Water Samples (June 2008): detects in 4 (18%) of 22 samples at a maximum concentration of 0.00358 µg/L and a median concentration of 0.003515 µg/L.
- City Road Drainage Ditch Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.0197 µg/L and a median concentration of 0.019 µg/L.
- Rice Lake Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.0179 µg/L and a median concentration of 0.0152 µg/L.
- *Albany, New York Rain, Snow, Surface Runoff, and Lake Samples (2006 – 2007)*: concentrations from 11 lake water samples ranged from 0.00115 – 0.0127 µg/L with a median concentration of 0.00409 µg/L; concentrations from 11 rain water samples ranged from less than the Limit of Quantitation (LOQ) – 0.00232 µg/L with a median concentration of 0.00056 µg/L; concentrations from 21 snow samples ranged from < LOQ – 0.00161 µg/L with a median concentration of 0.00039 µg/L; concentrations from 14 surface runoff samples ranged from < LOQ – 0.00644 µg/L with a median concentration of 0.00113 µg/L (Kim and Kannan, 2007).
- *Cape Fear Drainage Basin in North Carolina (2006)*: 100 water samples were collected from 80 different sites; detected above the LOQ (0.001 µg/L) in 55.7% of the samples; a maximum concentration of 0.329 µg/L and a median concentration of 0.0148 µg/L (Nakayama et al., 2007).

Persistence & Mobility

- No data for persistence and mobility.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

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UCMR 3 Analyte Information Sheet

Perfluorobutanesulfonic Acid (PFBS)

CASRN: 375-73-5

Background & Use

- Perfluorobutanesulfonic acid is a manmade chemical and is used in products to make them stain, grease, heat, and water resistant.
- Names & Synonyms: Perfluorobutanesulfonic acid; PFBxS; 1-perfluorobutanesulfonic acid; nonafluorobutanesulfonic acid.

Health Effects

- *Reference Dose (RfD)*: 0.0014 mg/kg/day, based on a No Observed Adverse Effect Level (NOAEL) of 60 mg/kg/day and an Uncertainty Factor (UF) of 300, and associated with decreased hemoglobin and hematocrit and histological changes in kidney (*Minnesota Department of Health, 2009*).
- *Minimal Risk Level (MRL)*: Not available.
- *NOAEL*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: Not available.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 9.8 µg/L for non-cancer effects in drinking water based on the RfD of 0.0014 mg/kg/day.
- *CDC's 95th Percentile Concentration*: Less than the limit of detection for 2,094 serum samples tested from 2003 – 2004 (*Calafat et al., 2007*).

Production & Release

- No data for production and release.

Occurrence in Water

- *Cape Fear Drainage Basin in North Carolina (2006)*: 100 water samples were collected from 80 different sites; detected above the Limit of Quantitation (LOQ) (0.001 µg/L) in 39.2% of the samples; a maximum concentration of 0.00941 µg/L and a median concentration of 0.00246 µg/L (*Nakayama et al., 2007*).
- *Minnesota's Ambient Environment (2006 – 2008)* (*Minnesota Pollution Control Agency, 2008*):
 - Rural Ambient Shallow Ground Water (October 2007): not detected in the 22 samples.

- Urban Ambient Shallow Ground Water (2006 – 2007): detects in 5 (17%) of 29 samples at a maximum concentration of 0.0399 µg/L and a median concentration of 0.00705 µg/L (includes concentrations less than the reporting level of 0.0025 µg/L).
- Mississippi and Minnesota River and Tributaries Water Samples (April 2008): detects in 1 (3%) of 34 samples at a concentration of 0.0162 µg/L (estimated value).
- Mississippi and Minnesota River Water Samples (August 2008): detects in 5 (14%) of 35 samples at a maximum concentration of 0.0878 µg/L and a median concentration of 0.0136 µg/L.
- Surface Water Samples (2006): detects in 3 (19%) of 16 samples at a maximum concentration of 0.0671 µg/L and a median concentration of 0.0552 µg/L.
- Brainerd Area Mississippi River Surface Water Samples (2007): detects in 2 (25%) of 8 samples at concentrations of 0.0202 and 0.026 µg/L.
- Mississippi River Surface Water Samples (June 2008): not detected in the 22 samples.
- City Road Drainage Ditch Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.0484 µg/L and a median concentration of 0.0429 µg/L.
- Rice Lake Surface Water Samples (2008): detects in 3 (100%) of 3 samples at a maximum concentration of 0.0286 µg/L and a median concentration of 0.0275 µg/L.

Persistence & Mobility

- No data for persistence and mobility.

References

Calafat A.M., L.Y. Wong, Z. Kuklenyik, J.A. Reidy, and L.L. Needham. 2007. Polyfluoroalkyl chemicals in the U.S. population: Data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons to NHANES 1999–2000. *Environmental Health Perspectives*. 115(11): 1578-1583.

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Minnesota Pollution Control Agency. 2008. *PFCs in Minnesota's Ambient Environment*. 2008 Progress Report.

Nakayama, S., M.J. Strynar, L. Helfant, P. Egeghy, X. Ye, and A.B. Lindstrom. 2007. Perfluorinated compounds in the Cape Fear Drainage Basin in North Carolina. *Environmental Science and Technology*. 41(15): 5271-5276.

UCMR 3 Analyte Information Sheet

Chromium (total) (regulated)

CASRN: 18540-29-9 (hexavalent chromium) and 16065-83-1 (trivalent chromium)

Chromium-6 (Hexavalent Chromium)

CASRN: 18540-29-9

Background & Use

Chromium (total)

- Chromium is a naturally-occurring element. The MCL of 0.1 mg/L covers the two forms primarily found in the environment: trivalent chromium (chromium-3) and hexavalent chromium (chromium-6). Chromium is used in making steel and other alloys. Chromium-3 or -6 forms are used for chrome plating, dyes and pigments, leather tanning, and wood preservation. Chromium-3 is an essential nutrient.
- Names & Synonyms: Chrome; chromium metal; Cr.

Chromium-6

- Chromium-6 is the highest oxidation state of the element chromium. Although chromium-6 can be formed by the oxidation of chromium-3, the primary mode of chromium-6 occurrence in the environment is via the release of industrial chemicals containing chromium-6.
- Names & Synonyms: Hexavalent chromium; chromium⁶⁺; chromium(VI); Cr-6; Cr VI.

Health Effects

Chromium (total)

- The current NPDWR establishes an MCL for total chromium; however, the Integrated Risk Information System (IRIS) Reference Dose (RfD) from 1998 for chromium-6 is the basis of the current Maximum Contaminant Level Goal (MCLG) because that is the more toxic species. The Maximum Contaminant Level (MCL) equals the MCLG for total chromium.

Chromium-6

- RfD: 0.005 mg/kg-day (*IRIS, 1998*).
- RfD: 0.003 mg/kg-day based on a No Observed Adverse Effect Level (NOAEL) of 2.5 mg/kg-day and an Uncertainty Factor (UF) of 300 in rats (*IRIS, 2005*).
- Draft RfD: 0.0009 mg/kg-day based on benchmark dose lo (BMDL) of 0.09 mg associated with incidence of diffuse epithelial hyperplasia of the duodenum (*IRIS, Draft Toxicological Review Released for External Review and public comment September 30, 2010; 75 FR 60454*).
- Minimal Risk Level (MRL): Not available.
- NOAEL: Not available.
- Lowest Observed Adverse Effect Level (LOAEL): Not available.

- *Draft Slope Factor*: $0.5 \text{ (mg/kg-day)}^{-1}$ based on the incidence of neoplasms in the small intestine of male mice (IRIS, *Draft Toxicological Review Released for External Review and public comment September 30, 2010*; 75 FR 60454).
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*:
 - Listed (*State of California List of Chemicals Known to Cause Cancer*).
 - D – not classifiable as to human carcinogenicity (*EPA Cancer Class*).
 - Clear evidence of carcinogenic activity (*NTP, 2008*).
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*:
 - $21 \text{ }\mu\text{g/L}$ for non-cancer effects in drinking water based on the RfD of 0.003 mg/kg-day .
 - $6.3 \text{ }\mu\text{g/L}$ for non-cancer effects in drinking water based on the draft RfD of 0.0009 mg/kg-day .
 - $0.7 \text{ }\mu\text{g/L}$ for cancer effects in drinking water based on the draft slope factor of $0.5 \text{ (mg/kg-day)}^{-1}$ (*set at 10^{-5} risk level*).

Production & Release

*Chromium (total)*¹

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: not reported.
- *Toxics Release Inventory (TRI) 2002*: facilities reported 17,299 pounds were released into surface water across 32 states, and a total of 10,021,057 pounds were released into the environment across 50 states.
- *TRI 2004*: facilities reported 19,940 pounds were released into surface water in 35 states, and a total of 10,802,415 pounds were released into the environment across 50 states.
- *TRI 2006*: facilities reported 9,391 pounds were released into surface water in 31 states, and a total of 11,452,248 pounds were released into the environment across 50 states.

Chromium-6

- No data for production and release.

Occurrence in Water

Chromium (total)

- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - Detects in 28,502 (15.33%) of 185,952 samples and in 11,840 (24.21%) of 48,908 systems at a maximum concentration of 5.2 mg/L and a median concentration of 0.00415 mg/L (percentages rounded to nearest hundredth).

¹ The NPDWR defines chromium (total) as the sum of chromium-3 and chromium-6. The TRI definition for total chromium also includes chromium-0.

- Forty-five states submitted data; total chromium was detected at levels above the MCL in 17 of those states.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 2,809 (47.2%) of 5,951 samples and at 2,068 (61.1%) of the 3,385 sites at a maximum concentration of 148 µg/L and a median concentration of 2 µg/L.
- *Wisconsin Water Quality Monitoring (2011)*: detects in 16 (100%) of 16 wells at a maximum concentration of 2.03 µg/L.

Chromium-6

- *Wisconsin Water Quality Monitoring (2011)*: detects in 13 (81%) of 16 wells at a maximum concentration of 1.79 µg/L (of 2.03 µg/L total chromium).
- *EWG Tap Water Study (2010)*: detects in 31 (89%) of 35 samples at a maximum concentration of 12.9 µg/L and a median concentration of 0.18 µg/L.

Persistence & Mobility

- The two most prevalent forms of chromium in the environment, chromium-3 and chromium-6, exist in both water-soluble and insoluble forms. Soluble forms of chromium-3 and chromium-6 can be interconverted via redox transformation, which is highly pH-dependent.
- The nature of chromium that is present in water is dependent upon precipitation/dissolution and adsorption/desorption processes, which are also pH-dependent. In contrast to chromium-6, the adsorption of chromium-3 on suspended solids and sediment increases as pH increases.
- Chromium-6 predominates under highly oxidizing conditions; whereas chromium 3 predominates under reducing conditions. The reduction half-life of chromium-6 in water with sediment ranged from 4 to 140 days. Dissolved oxygen by itself in natural waters does not cause any measurable oxidation of chromium-3 to chromium-6 in 128 days. Therefore, oxidation of chromium-3 will not be significant in most natural waters.

References

EWG. 2010. *Chromium-6 in U.S. Tap Water*. Available on the Internet at:
<http://www.ewg.org/chromium6-in-tap-water>.

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Appendix A – Persistence and Mobility

Persistence and mobility are defined by chemical properties that measure or estimate environmental fate characteristics of a contaminant and affect their likelihood to occur in the water environment. There are a number of data elements that measure the fate of a chemical in the environment. The physical and chemical parameters that are most relevant to their fate in drinking water are summarized in Table 1. The data elements listed in the table are arranged in hierarchical order, with the most important at the top. The scales used to categorize persistence and mobility were recommended by the National Drinking Water Advisory Committee (NDWAC) CCL 3 workgroup. The approach was developed by implementing parts of the recommendations of the National Research Council (NRC) and using testing protocols developed by the NDWAC's CCL 3 workgroup. The persistence and mobility data are arrayed into low-medium-high categories as suggested by NRC. The categories are given values of 1 (not very mobile), 2 (moderately mobile), or 3 (very mobile) based on the ranking of the measurement from low to high. Since the persistence and mobility data are being used as a measure of magnitude, a low ranking (1) for a parameter is one that will minimize the concentration in water and a high ranking (3) is one that will maximize the concentration.

Table 1. Magnitude Scales for Environmental Fate Data¹

Magnitude Hierarchy 5

Mobility Scale

	Units	Value		
		1 (Low)	2 (Medium)	3 (High)
Organic Carbon Partitioning Coefficient (K_{oc})	mL/g	> 1,000	100-1,000	< 100
Octanol-Water Partitioning Coefficient ($\log K_{ow}$)	Dimensionless	> 4	1-4	< 1
Henry's Law Coefficient (K_H)	atm-m ³ /mol	> 10 ⁻³	10 ⁻⁷ -10 ⁻³	< 10 ⁻⁷
Water Solubility	mg/L	< 1	1-1,000	> 1,000
Percent in Water in a Water/Air/Soil/Sediment System (W%) (PBT Profiler)	Dimensionless	≤ 25	> 25-50	> 50

Persistence Scale

	Units	Value		
		1 (Low)	2 (Medium)	3 (High)
Half Life ($t_{1/2}$)	Time	Days, days-weeks	Weeks, weeks-months	Months, recalcitrant
Measured Degradation Rate ²	Time	Days, days-weeks (BF, BFA) ³	Weeks, weeks-months (BS, BSA)	Months, recalcitrant (BST)
Modeled Degradation Rate (PBT Profiler)	Time	Days, days-weeks	Weeks, weeks-months	Months, recalcitrant

¹ Table 1 was modified from Exhibit A.8 in *Final Contaminant Candidate List 3 Chemicals: Classification of the PCCL to CCL* (EPA 815-R-09-008, August, 2009).

² When two results are found for a measured degradation rate, the data are "averaged" and then a value is determined.

³ BF = Biodegrades Fast, BFA = Biodegrades Fast with Acclimation, BS = Biodegrades Slow, BSA = Biodegrades Slow with Acclimation, BST = Biodegrades Sometimes.

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Appendix B – List of Chemical Contaminants Considered for Inclusion on UCMR 3

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
630-20-6	1,1,1,2-Tetrachloroethane			X				A
75-34-3	1,1-Dichloroethane	X	X	X			X	
96-18-4	1,2,3-Trichloropropane			X			X	
122-66-7	1,2-Diphenylhydrazine	X	X		SS ⁶			C
106-99-0	1,3-Butadiene			X			X	
99-65-0	1,3-Dinitrobenzene			X		AM ⁷		D
123-91-1	1,4-Dioxane			X			X	
50-27-1	Estriol			X			X	
57-91-0	17- α -Estradiol			X				B
57-63-6	17- α -Ethinylestradiol			X			X	
50-28-2	17- β -Estradiol			X			X	
71-36-3	1-Butanol			X				B
88-06-2	2,4,6-Trichlorophenol	X	X		SS			C
120-83-2	2,4-Dichlorophenol	X	X		SS			C
51-28-5	2,4-Dinitrophenol	X	X		SS			C
109-86-4	2-Methoxyethanol			X				B
95-48-7	2-Methyl-phenol (o-Cresol)	X	X		SS			C
107-18-6	2-Propen-1-ol		z	X				B
16655-82-6	3-Hydroxycarbofuran			X				A
101-77-9	4,4'-Methylenedianiline			X				B
63-05-8	4-Androstene-3,17-dione						X	
521-18-6	5- α -Dihydrotestosterone							E
30560-19-1	Acephate			X				E
75-07-0	Acetaldehyde			X				A
60-35-5	Acetamide			X				B
34256-82-1	Acetochlor	X	X	X	AM	SS		C, D
187022-11-3	Acetochlor ethanesulfonic acid (ESA)			X		SS		D

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
194992-44-4	Acetochlor oxanilic acid (OA)			X		SS		D
107-02-8	Acrolein			X				B
142363-53-9	Alachlor ethanesulfonic acid (ESA)	X	X	X		SS		D
171262-17-2	Alachlor oxanilic acid (OA)			X		SS		D
319-84-6	alpha-Hexachlorocyclohexane			X				F
64285-06-9	Anatoxin-a			X				E
62-53-3	Aniline			X				B
741-58-2	Bensulide			X				B
100-44-7	Benzyl chloride			X				B
80-05-7	Bisphenol A (4,4'-Isopropylidenediphenol)							E
74-97-5	Bromochloromethane (Halon 1011)			X			X	
74-83-9	Bromomethane (Methyl bromide)	X	X	X			X	
25013-16-5	Butylated hydroxyanisole			X				B
133-06-2	Captan			X				E
298-46-4	Carbamazepine							E
14866-68-3	Chlorate			X			X	
75-45-6	Chlorodifluoromethane (HCFC-22)			X			X	
74-87-3	Chloromethane (Methyl chloride)			X			X	
110429-62-4	Clethodim			X				E
7440-48-4	Cobalt			X			X	
80-15-9	Cumene hydroperoxide			X				B
143545-90-8	Cylindrospermopsin			X				E
18540-29-9	Chromium-6 ⁹						X	
17040-19-6	Demeton-S-methyl sulfone							E
333-41-5	Diazinon	X	X		SS			C
141-66-2	Dicrotophos			X				E
55290-64-7	Dimethipin			X				E
60-51-5	Dimethoate			X		AM		D

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
298-04-4	Disulfoton	X	X	X	SS			C
330-54-1	Diuron	X	X	X	SS			C
517-09-9	Equilenin			X				B
474-86-2	Equilin			X			X	
114-07-8	Erythromycin			X				B
53-16-7	Estrone			X			X	
563-12-2	Ethion							E
13194-48-4	Ethoprop			X				F
107-21-1	Ethylene glycol			X				B
75-21-8	Ethylene oxide			X				B
96-45-7	Ethylene thiourea			X				E
22224-92-6	Fenamiphos			X				F
31972-44-8	Fenamiphos sulfone							E
31972-43-7	Fenamiphos sulfoxide							E
54910-89-3	Fluoxetine							E
944-22-9	Fonofos	X	X		SS			C
50-00-0	Formaldehyde			X				A
7440-56-4	Germanium			X				B
110-54-3	Hexane			X				B
302-01-2	Hydrazine			X				B
330-55-2	Linuron	X	X		SS			C
72-33-3	Mestranol			X				B
10265-92-6	Methamidophos			X				E
67-56-1	Methanol			X				B
16752-77-5	Methomyl							E
1634-04-4	Methyl tert-butyl ether	X	X	X	AM			C
51218-45-2	Metolachlor	X	X	X		SS		D
171118-09-5	Metolachlor ethanesulfonic acid (ESA)			X		SS		D

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
152019-73-3	Metolachlor oxanilic acid (OA)			X		SS		D
101043-37-2	Microcystin-LR			X				E
2212-67-1	Molinate	X	X	X	AM			C
7439-98-7	Molybdenum			X			X	
	N-ethyl perfluorooctanesulfonamido-acetic acid (NEtFOSAA)							E
98-95-3	Nitrobenzene	X	X	X	SS & AM			C
1836-75-5	Nitrofen							F
55-63-0	Nitroglycerin			X				B
	N-methyl perfluorooctanesulfonamido-acetic acid (NMeFOSAA)							E
872-50-4	N-Methyl-2-pyrrolidone			X				B
55-18-5	N-nitrosodiethylamine (NDEA)			X		SS		D
62-75-9	N-nitrosodimethylamine (NDMA)			X		SS		D
621-64-7	N-nitroso-di-n-propylamine (NDPA)			X		SS		D
86-30-6	N-nitrosodiphenylamine			X				B
930-55-2	N-nitrosopyrrolidine (NPYR)			X		SS		D
68-22-4	Norethindrone			X				B
103-65-1	<i>m</i> -Propylbenzene			X				G
95-53-4	<i>o</i> -Toluidine			X				E
75-56-9	Oxirane, methyl-			X				B
301-12-2	Oxydemeton-methyl			X				E
42874-03-3	Oxyfluorfen			X				E
14797-73-0	Perchlorate	X	X	X	AM			C
375-73-5	Perfluorobutanesulfonic acid (PFBS)						X	
335-76-2	Perfluorodecanoic acid (PFDA)							E
307-55-1	Perfluorododecanoic acid (PFDoA)							E
375-85-9	Perfluoroheptanoic acid (PFHpA)						X	
355-46-4	Perfluorohexanesulfonic acid (PFHxS)						X	
307-24-4	Perfluorohexanoic acid (PFHxA)							E
375-95-1	Perfluorononanoic acid (PFNA)						X	

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
1763-23-1	Perfluorooctanesulfonic (PFOS)			X			X	
335-67-1	Perfluorooctanoic acid (PFOA)			X			X	
376-06-7	Perfluorotetradecanoic acid (PFTA)							E
72629-94-8	Perfluorotridecanoic acid (PFTrDA)							E
2058-94-8	Perfluoroundecanoic acid (PFUnA)							E
52645-53-1	Permethrin			X				F
41198-08-7	Profenofos			X				E
57-83-0	Progesterone							E
1610-18-0	Prometon	X	X		SS			C
91-22-5	Quinoline			X				E
121-82-4	RDX (Hexahydro-1,3,5-trinitro-1,3,5-triazine)	X	X	X		AM		D
135-98-8	<i>sec</i> -Butylbenzene			X				G
7440-24-6	Strontium			X			X	
107534-96-3	Tebuconazole			X				E
112410-23-8	Tebufozide			X				B
13494-80-9	Tellurium			X				B
13071-79-9	Terbufos	X	X	X	SS			C
56070-16-7	Terbufos sulfone			X		AM		D
58-22-0	Testosterone						X	
59669-26-0	Thiodicarb			X				E
23564-05-8	Thiophanate-methyl			X				E
26471-62-5	Toluene diisocyanate			X				B
78-48-8	Tribufos			X				E
121-44-8	Triethylamine			X				B
76-87-9	Triphenyltin hydroxide (TPTH)			X				B
51-79-6	Urethane			X				B
7440-62-2	Vanadium	X	X	X			X	

CAS #	Contaminant	CCL 1 ¹	CCL 2 ²	CCL 3 ³	UCMR 1 ⁴	UCMR 2 ⁵	UCMR 3	Reason for exclusion from UCMR 3 ⁸
50471-44-8	Vinclozolin			X				F
137-30-4	Ziram			X				B

¹ USEPA. 1998. Announcement of the Drinking Water Contaminant Candidate List; Notice: March 2, 1998. Volume 63, Number 140: 10273-10287.

² USEPA. 2005. Drinking Water Contaminant Candidate List 2; Final Notice. Federal Register: February 24, 2005. Volume 70, Number 36: 9071-9077.

³ USEPA. 2009. Drinking Water Contaminant Candidate List 3--Final. Federal Register: October 8, 2009. Volume 74, Number 194: 51850-51862.

⁴ USEPA. 1999. Revisions to the Unregulated Contaminant Monitoring Regulation for Public Water Systems; Final Rule. Federal Register. Vol. 64, No. 180, p. 50556, September 17, 1999.

⁵ USEPA. 2007. Unregulated Contaminant Monitoring Regulation (UCMR) for Public Water Systems Revisions. Federal Register. Vol. 72, No. 2, p. 367, January 4, 2007.

⁶ SS = Screening Survey (List 2); includes contaminants measured using specialized analytical method technologies not commonly used by drinking water laboratories.

⁷ AM = Assessment Monitoring (List 1); includes contaminants measured with common analytical method technologies used by drinking water laboratories.

⁸ A = Lower priority than 30 UCMR 3 contaminants
 B = No method ready in time for rule
 C = Listed on UCMR 1
 D = Listed on UCMR 2
 E = Further evaluation of *Health Reference Level (HRL)* to *Minimal Risk Level (MRL)* ratio required
 F = Alternative method in development
 G = Proposed, but not included in the final rule.

⁹ While EPA did not include chromium-6 in the proposed list of chemicals for UCMR 3 monitoring, EPA did request comment on whether it should be included in the final rule due to concerns about its potential occurrence in public water supplies. EPA also requested comments on whether total chromium should be measured concurrent with chromium-6. Commenters strongly supported requiring monitoring for both chromium-6 and total chromium. EPA is using the authority provided in SDWA Section 1445(a)(1)(A) to require monitoring for total chromium in conjunction with the UCMR 3 monitoring of chromium-6.

Appendix C – Proposed Contaminants Removed for the Final UCMR 3

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Proposed UCMR 3 Analyte Information Sheet

sec-Butylbenzene

CASRN: 135-98-8

Background & Use

- *sec*-Butylbenzene is an alkylated aromatic compound. It is used as a solvent for coating compositions, in organic synthesis, and as a plasticizer and in surface active agents.
- Names & Synonyms: *sec*-Butylbenzene; (1-methylpropyl)benzene; 2-phenylbutane.
- *sec*-Butylbenzene is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 4.42 mg/kg/day, based on a 24-week study in rats, associated with behavioral changes, such as alteration of classic conditioning (*Registry of Toxic Effects of Chemical Substances [RTECS] Lowest Oral Chronic LOAEL*).
- *Hazardous Substances Data Bank (HSDB) Lowest Oral Lethal Dose (LD₅₀)*: 2,240 mg/kg.
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 10.3 µg/L for non-cancer effects in drinking water, based on the RTECS LOAEL of 4.42 mg/kg/day.

Production & Release

- No data for production and release.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD):
 - Round 1 (1988 – 1992): occurred at 28 (0.23%) of the 12,343 PWSs, at a maximum concentration of 19.8 µg/L and a median concentration of 0.7 µg/L.
 - Round 2 (1993 – 1997): occurred at 34 (0.15%) of the 22,974 PWSs, at a maximum concentration of 22 µg/L and a median concentration of 0.57 µg/L.

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 53 (4.17%) of 1,270 samples; detects were from 44 (7.65%) of the 575 sites; detects were from 3 states; detects ranged from 0.4 – 6.1 µg/L.
 - Surface Water: detects in 297 (47.90%) of 620 samples; detects were from 17 (13.93%) of the 122 sites; detects were from 3 states; detects ranged from 0.001 – 0.7 µg/L.
 - Ohio Public Water Supply: detect in 1 (0.08%) of 1,277 samples; detect was from 1 (0.54%) of the 186 sites; detect was from 1 (100%) state; detected concentration equaled 0.5 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 42 (0.71%) of 5,941 samples and at 25 (0.58%) of the 4,309 sites at a maximum concentration of 11 µg/L and a median concentration of 0.39 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water system (CWS) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; not detected at the reporting level of 0.2 µg/L (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 1.5% of the CWSs sampled (2.6% of ground water sites and 0% of surface water sites) at concentrations ranging from 0.05 – 0.07 µg/L (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 209 urban wells and 1,396 rural wells; 1.91% detection frequency in urban areas and 0.14% detection frequency in rural areas at concentrations ranging from 0.2 – 11 µg/L. In urban wells, the median concentration was 1.65 µg/L and in rural wells, the median concentration was 2.3 µg/L (Squillace et al., 1999) (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
- *Six-Year Data (1998 – 2005)*: supplemental contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:
 - California: detects in 9 (0.01%) of 114,109 drinking water samples; detects were from 8 (0.20%) of the 4,006 PWSs that reported data; detects ranged from 0.5 – 8.3 µg/L.
 - North Carolina: detects in 10 (0.05%) of 19,843 drinking water samples; detects were from 8 (0.32%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 9.5 µg/L.
 - Ohio: detects in 4 (0.04%) of 9,288 drinking water samples; detects were from 3 (0.12%) of the 2,533 PWSs that reported data; detects ranged from 0.5 – 2.1 µg/L.
 - South Dakota: not detected in 1,110 drinking water samples from 281 PWSs that reported data.
 - Texas: not detected in 36,284 drinking water samples from 5,660 PWSs that reported data.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 1 (0.04%) of 2,569 drinking water samples at a concentration of 1.3 µg/L; 1,056 PWSs sampled.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: not detected in 3,409 drinking water samples from 743 PWSs that reported data.

Persistence & Mobility

- *Water Solubility*: 17.6 mg/L, indicates sec-butylbenzene is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 7,200 L/kg, indicates sec-butylbenzene is not very mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 4.57, indicates sec-butylbenzene is not very mobile in water.
- *Henry's Law Constant (K_H)*: 0.0176 atm-m³/mol, indicates sec-butylbenzene is not very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System (W%)*: 15% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 15 days, indicates sec-butylbenzene is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

Grady, S.J. 2003. *A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4079, 85 p.

Squillace, P.J., M.J. Moran, W.W. Lapham, C.V. Price, R.M. Clawges, and J.S. Zogorski. 1999. Volatile Organic Compounds in Untreated Ambient Groundwater of the United States, 1985-1995. *Environmental Science and Technology*. 33(23): 4176-4187.

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Proposed UCMR 3 Analyte Information Sheet

n-Propylbenzene

CASRN: 103-65-1

Background & Use

- *n*-Propylbenzene is an alkylated aromatic compound used in the manufacture of methylstyrene, in textile dyeing, as a printing solvent, and is a constituent of asphalt and naptha.
- Names & Synonyms: *n*-Propylbenzene; Benzene, propyl-; 1-phenylpropane; propylbenzene.
- *n*-Propylbenzene is one of 104 chemicals on CCL 3.

Health Effects

- *Reference Dose (RfD)*: Not available.
- *Minimal Risk Level (MRL)*: Not available.
- *No Observed Adverse Effect Level (NOAEL)*: Not available.
- *Lowest Observed Adverse Effect Level (LOAEL)*: 2.5 mg/kg/day, based on a 24-week study in rats, and associated with effects on the blood, such as changes in the spleen (*Registry of Toxic Effects of Chemical Substances [RTECS] Lowest Oral Chronic LOAEL*).
- *RTECS Lowest Oral Lethal Dose (LD₅₀)*: 6,040 mg/kg, based on a study in rats, associated with behavioral effects, such as somnolence (general depressed activity).
- *Slope Factor*: Not available.
- *Acceptable Daily Intake (ADI)*: Not available.
- *Cancer and/or Teratogen Class*: Not available.
- *Drinking Water Equivalent Level (DWEL)*: Not available.
- *Health Reference Level (HRL)*: 5.83 µg/L for non-cancer effects in drinking water based on the RTECS LOAEL of 2.5 mg/kg/day.

Production & Release

- *Chemical Update System/Inventory Update Rule (CUS/IUR)*: production was approximately > 10,000 – 500,000 pounds in 1998 and in 2002.

Occurrence in Water

- *Unregulated Contaminant Monitoring (UCM) Data*: analytical results for samples collected by public water systems (PWSs) from 1988 – 1997 for (then) unregulated contaminants; datasets are stored in EPA's National Contaminant Occurrence Database (NCOD).
 - Round 1 (1988 – 1992): occurred at 42 (0.33%) of the 12,724 PWSs, at a maximum concentration of 34 µg/L and a median concentration of 0.7 µg/L.
 - Round 2 (1993 – 1997): occurred at 54 (0.24%) of the 22,970 PWSs, at a maximum concentration of 21 µg/L and a median concentration of 0.6 µg/L.

- *EPA's Storage and Retrieval (STORET) Database (1999 – Present)*: data submission to STORET is voluntary; the extent of national coverage and data completeness may vary.
 - Ground Water: detects in 67 (5.14%) of 1,303 samples; detects were from 46 (7.78%) of the 591 sites; detects were from 3 states; detects ranged from 0.5 – 390 µg/L.
 - Surface Water: detects in 266 (43.54%) of 611 samples; detects were from 17 (13.60%) of the 125 sites; detects were from 3 states; detects ranged from 0.001 – 1.7 µg/L.
 - Ohio Public Water Supply: detect in 1 (0.08%) of 1,277 samples; detect was from 1 (0.54%) of the 186 sites; detect was from 1 (100%) state; detected concentration equaled 0.5 µg/L.
- *National Water-Quality Assessment (NAWQA) Program (1992 – 2001)*: detects in 90 (1.51%) of 5,941 samples and at 53 (1.23%) of the 4,309 sites at a maximum concentration of 47 µg/L and a median concentration of 0.024 µg/L.
- *NAWQA Volatile Organic Compound (VOC) National Synthesis Random and Focused VOC Surveys*: random survey designed to be nationally representative of community water systems (CWSs) source water and focused survey designed to provide insight into temporal variability and anthropogenic factors associated with VOC occurrence. (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
 - Random Survey (1999 – 2000): samples taken from the source waters of 954 CWSs; detects in 1 (0.10%) of the samples (0% of ground water samples and 0.27% of surface water samples) at a concentration of 0.21 µg/L (Grady, 2003).
 - Focused Survey (1999 – 2001): 451 samples taken from source waters serving 134 CWSs; detected at 0.8% of the CWSs sampled (1.3% of ground water sites and 0% of surface water sites). Below the reporting level of 0.2 µg/L, detected at 3.0% of the CWSs sampled (1.3% of ground water sites and 5.4% of surface water sites). Concentrations ranged from 0.05 – 0.47 µg/L (Delzer and Ivahnenko, 2003).
- *NAWQA VOC National Synthesis Compilation of Historical VOC Monitoring Data (1985 – 1995)*: samples taken from 241 urban wells and 1,462 rural wells; 2.07% detection frequency in urban areas and 0.21% detection frequency in rural areas at concentrations ranging from 0.6 – 47 µg/L. In urban wells, the median concentration was 4.5 µg/L and in rural wells, the median concentration was 1.9 µg/L (Squillace et al., 1999). (Note: language in the referenced literature is ambiguous with respect to samples vs. sites.)
- *NAWQA VOCs in Ground Water and Drinking Water Supply Wells (1985 – 2001)*: national assessment comprised of approximately 100 different aquifer studies; roughly 3,500 water samples collected from various types of wells:
 - Aquifers: detects in 1 (0.041%) of 2,461 samples at a concentration of 0.048 µg/L.
 - Shallow ground water in urban areas: detects in 8 (0.9%) of 847 samples.
 - Shallow ground water in agricultural areas: detects in 1 (0.1%) of 721 samples.
 - Domestic wells: detects in 1 (0.052%) of 1,932 samples at a concentration of 0.061 µg/L.
 - Public wells: not detected in 950 samples.
 - Domestic and public wells: detects in 1 (< 0.1%) of 2,882 samples.
- *Six-Year Data (1998 – 2005)*: contaminant occurrence data voluntarily submitted by states to EPA in support of national contaminant occurrence assessments conducted for the second Six-Year Review:

- California: detects in 12 (0.01%) of 115,072 drinking water samples; detects were from 9 (0.22%) of the 4,033 PWSs that reported data; detects ranged from 0.52 – 4.5 µg/L.
- North Carolina: detects in 14 (0.07%) of 19,831 drinking water samples; detects were from 11 (0.44%) of the 2,493 PWSs that reported data; detects ranged from 0.5 – 3.8 µg/L.
- Ohio: detects in 4 (0.04%) of 9,288 drinking water samples; detects were from 4 (0.16%) of the 2,533 PWSs that reported data; detects ranged from 0.56 – 1.8 µg/L.
- Texas: detects in 6 (0.02%) of 36,284 drinking water samples; detects were from 5 (0.09%) of the 5,660 PWSs that reported data; detects ranged from 1.1 – 6.8 µg/L.
- *Wisconsin Department of Natural Resources (1983 – 1999)*: detects in 1 (0.04%) of 2,580 drinking water samples at a concentration of 1.9 µg/L; 1,062 PWSs sampled.
- *Wisconsin Department of Natural Resources (2000 – 2009)*: detects in 1 (0.03%) of 3,303 drinking water samples at a concentration of 1.1 µg/L; 741 PWSs sampled.

Persistence & Mobility

- *Water Solubility*: 52.2 mg/L, indicates n-propylbenzene is moderately mobile in water.
- *Organic Carbon Partitioning Coefficient (K_{oc})*: 955 L/kg, indicates n-propylbenzene is moderately mobile in water.
- *Octanol-Water Partitioning Coefficient ($\log K_{ow}$)*: 3.69, indicates n-propylbenzene is moderately mobile in water.
- *Henry's Law Constant (K_H)*: 0.0105 atm·m³/mol, indicates n-propylbenzene is not very mobile in water.
- *Percent in Water in a Water/Air/Soil/Sediment System ($W\%$)*: 22% (PBT Profiler).
- *Estimated Biodegradation Half-Life*: 15 days, indicates n-propylbenzene is moderately persistent in the environment.

References

Delzer, G.C. and T. Ivahnenko. 2003. *Occurrence and Temporal Variability of Methyl tert-Butyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4084, 65 p.

Grady, S.J. 2003. *A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey*. U.S. Geological Survey Water-Resources Investigations Report 02-4079, 85 p.

Squillace, P.J., M.J. Moran, W.W. Lapham, C.V. Price, R.M. Clawges, and J.S. Zogorski. 1999. Volatile Organic Compounds in Untreated Ambient Groundwater of the United States, 1985-1995. *Environmental Science and Technology*. 33(23): 4176-4187.